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# Outdoor Smog Chamber Experiments Reactivity of Methanol Exhaust Part 2. Quality Assurance and Data Processing System Description

North Carolina Univ. at Chapel Hill

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This report describes the Quality Assurance and Data Processing procedures and systems used at the UNC Outdoor Smog Chamber Facility. The primary product of research conducted at this facility is information in the form of measurements of reactants and products in photochemical systems and measurements of the critical parameters that influence the chemical transformations system.

Generating useful data begins with understanding the goals of the project and the special needs and concerns of conducting a successful smog chamber operation. The system components are designed to collect, transfer, process, and report accurate, high resolution data without loss or distortion. The system components in the Quality Assurance and Data Processing system are: people, hardware, software, checklists, and data bases.

Quality assurance checks are made at every level of the program. Pressurized gas tank and liquid mixtures were used to establish experimental conditions of HC assuring consistency throughout the program. Several NBS traceable standards and liquid injections into the chamber used for calibration have been intercompared and show good agreement. Resulting calibration data indicates good instrument stability during the program.

The document describes the calibration techniques and data processing procedures, and the processing of experimental data. A description and examples of the format of the final documentation and data file are given. The last chapter summarizes the Quality Assurance steps and important accuracy and precision aspects of the data quality.

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H. E. Jeffries, K. G. Sexton,
R. M. Kamens, M. S. Holleman

Department of Environmental Sciences
and Engineering
School of Public Health
University of North Carolina
Chapel Hill, N.C. 27514

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Technical Representative: Penny M. Carey

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Ann Arbor, MI 48105

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# Abstract

This report describes the Quality Assurance and Data Processing procedures and systems used at the UNC Outdoor Smog Chamber Facility. The primary product of research conducted at this facility is information in the form of measurements of reactants and products in photochemical systems and measurements of the critical parameters that influence the chemical transformations system.

Generating useful data begins with understanding the goals of the project and the special needs and concerns of conducting a successful smog chamber operation. The system components are designed to collect, transfer, process, and report accurate, high resolution data without loss or distortion. The system components in the Quality Assurance and Data Processing system are: people, hardware, software, checklists, and data bases.

Quality assurance checks are made at every level of the program. Pressurized gas tank and liquid mixtures were used to establish experimental conditions of HC assuring consistency throughout the program. Several NBS traceable standards and liquid injections into the chamber used for calibration have been intercompared and show good agreement. Resulting calibration data indicates good instrument stability during the program.

The document describes the calibration techniques and data processing procedures, and the processing of experimental data. A description and examples of the format of the final documentation and data file are given. The last chapter summarizes the Quality Assurance steps and important accuracy and precision aspects of the data quality.

# Contents

1 Overall QA Steps 1

Introduction . . . . . 1

Clearly Established Goals . . . . . 1

Facilities and Analytical Support Requirements . . . . . 2

Planning of Activities . . . . . 2
- Calibrations . . . . . 2
- Characterization Runs . . . . . 2
- Special Mixtures . . . . . 5
- Special Techniques . . . . . 5

Reviewing and Scheduling Methods . . . . . 5
- Priority of Runs . . . . . 5
- Use of NOAA Weather Radio . . . . . 5
- Feedback Scheduling . . . . . 6

Site Operation . . . . . 6
- Lab Air Conditioner . . . . . 6
- Smog Chamber . . . . . 7
- Chamber Sampling Manifold . . . . . 7
- Chamber AC Drying System . . . . . 7
- Ethylene Convertor . . . . . 7
- Mass Balance . . . . . 7
- Supplies . . . . . 8

Check Lists . . . . . 8
- Setup Checkout Lists . . . . . 8
- Operator Checkout List . . . . . 8
- Run Checkout List . . . . . 8
- Run Packup List . . . . . 8

Preventative Maintenance . . . . . 9

Characterization Experiments . . . . . 9
- Types of Characterization Experiments . . . . . 9
- Frequency . . . . . 10

**2 System Components** 11

**Location of Work** 11
- Experimental Site 11
- Data Processing Location 11

**Personnel** 12
- Advisory Group, AG 12
- Administrative Research Assistant, AA 12
- Project Coordinator, PC 12
- Site Operator, SO 12
- Peak Picker, PP 12
- Computer Technician, CT 12

**Computers Used** 12
- DEC PDP-11/40 13
- DEC LSI-11/23 13
- IBM PC 13
- DEC VAX-11/780 13

**Computer Programs Used** 14
- Description of General Purpose Programs 14
- Description of Specific Programs 14

**Description of Data File Formats and Contents** 15
- "U" file 15
- "G" file 15
- "P" files 16
- "C" files 16
- "K" files 17
- "R" files 17
- "Q" files 17
- "A" files 17
- "E" files 17
- ACDTR.COM file 17

**Description of Databases** 17

**Description of Database Procedures** 18
- List of all DTR Procedures by Name and Function 18
- Worksheets/Databases 19

**3 Calibration** 21

**Approach** 21

**NBS-Traceable Sources** . . . . . . . . . . . . . . . . . . . . . . . 21
NO and O3 Sources . . . . . . . . . . . . . . . . . . . . . . . 21
Hydrocarbon Sources . . . . . . . . . . . . . . . . . . . . . . . 22
Transfer Standards Created from Primary Sources . . . . . . . . . . . 23

**Primary Source Comparison** . . . . . . . . . . . . . . . . . . . . . 23
NO and O3 Sources . . . . . . . . . . . . . . . . . . . . . . . 23
Hydrocarbon Sources . . . . . . . . . . . . . . . . . . . . . . . 27

**Transfer Calibration to working "AUTOCAL" Sources** . . . . . . . . . . . 27
NOx and O3 Calibration Sources . . . . . . . . . . . . . . . . . . 27
Manual Gas Phase Titration . . . . . . . . . . . . . . . . . . . 27
Hydrocarbon Sources . . . . . . . . . . . . . . . . . . . . . . . 31

**Routine NOx and O3 Calibrations Methods** . . . . . . . . . . . . . . . 40
Automatic Source Sampling . . . . . . . . . . . . . . . . . . . . 40

**Routine HC Calibrations** . . . . . . . . . . . . . . . . . . . . . . 40
Automatic Source Sampling . . . . . . . . . . . . . . . . . . . . 41
Manual Precision Liquid Injections . . . . . . . . . . . . . . . . . 41

**Meteorological Sensor Calibrations** . . . . . . . . . . . . . . . . . . 42
Solar/UV radiation Calibrations . . . . . . . . . . . . . . . . . . 42
Temperature Calibrations . . . . . . . . . . . . . . . . . . . . . 42
Dewpoint Calibrations . . . . . . . . . . . . . . . . . . . . . . 42

**Flowrate Measurements - Calibration** . . . . . . . . . . . . . . . . . 43

**Time Measurement - Clock Calibration** . . . . . . . . . . . . . . . . . 43

**Calibration Documentation and Processing Databases** . . . . . . . . . . . 43
Paper Forms . . . . . . . . . . . . . . . . . . . . . . . . . . 43
Electronic Forms and Other Documentation . . . . . . . . . . . . . . 44
Calibration Data Processing Status Database (CALENTRY . . . . . . . . . . . 48
Calibration Databases . . . . . . . . . . . . . . . . . . . . . . 48
Security of Calibration Databases . . . . . . . . . . . . . . . . . 52

**Calibration Data Processing** . . . . . . . . . . . . . . . . . . . . 53
$NO_x$ and $O_3$ . . . . . . . . . . . . . . . . . . . . . . . . 53
HC Processing . . . . . . . . . . . . . . . . . . . . . . . . . 54

**4 Experimental Data** 71

Experimental Results Documentation . . . 71
  Data . . . 71
  Forms . . . 73
  Plots . . . 77
  Run Data Processing Status Databases . . . 77

Description of Data Processing Status Database . . . 89
  Description . . . 89
  Use of Data Processing Status Database . . . 89

Digital Voltmeter Data Processing . . . 91

Strip Chart Data Processing . . . 95

Documentation Processing . . . 99
  General Documentation Form . . . 100
  General Description and Purpose of Experiment . . . 100
  Initial Conditions . . . 100
  Meteorological Conditions . . . 102
  Data Times, Data Exceptions, Special Problems and Concerns . . . 102
  Quality Assessment . . . 102
  Documentation File Production . . . 104

Final Segmented File Production . . . 105

Security of Data . . . 107
  Inventory . . . 107
  Retention of Data . . . 107
  Backup of Data . . . 107

5 Segmented Data File 108

General Description . . . 108

File Formats . . . 109

ANSI Tape File Format . . . 112

Tape Contents . . . 113

Final Data Plots made from SegFile . . . 113

6 Summary of QA 124

Summary of Calibration and Data QA . . . . . . . . . . . . . . . . . . . . 124

List of QA Steps . . . . . . . . . . . . . . . . . . . . . . . . . . . . 125
  Before Runs . . . . . . . . . . . . . . . . . . . . . . . . . . . . 125
  After Run-Experiment Logging . . . . . . . . . . . . . . . . . . . . 125
  During Calibration . . . . . . . . . . . . . . . . . . . . . . . . . 126
  During DVM Data Processing . . . . . . . . . . . . . . . . . . . . . 127
  During GC Data Processing . . . . . . . . . . . . . . . . . . . . . 128
  During Documentation Stages . . . . . . . . . . . . . . . . . . . . 129
  After SegFile Made . . . . . . . . . . . . . . . . . . . . . . . . 130

APPENDICES

A Site Checklists 132

Checklist For 0900 EDT Site Operator. . . . . . . . . . . . . . . . . . 132
  Outside Check . . . . . . . . . . . . . . . . . . . . . . . . . . . 132
  TSR and UV zero check . . . . . . . . . . . . . . . . . . . . . . . 135
  GC Check . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 135

Checklist for Leaving the Site Set Up for a Run . . . . . . . . . . . . . 137
  Computer . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 137
  Formaldehyde . . . . . . . . . . . . . . . . . . . . . . . . . . . 137
  NOx and O3 Instruments . . . . . . . . . . . . . . . . . . . . . . 137
  TSR and UV Chart . . . . . . . . . . . . . . . . . . . . . . . . . 138
  Charts . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 138
  Carle I . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 139
  Carle II and Carle III . . . . . . . . . . . . . . . . . . . . . . 139
  Sigma 10 Integrator . . . . . . . . . . . . . . . . . . . . . . . . 140
  Dew Point Meter . . . . . . . . . . . . . . . . . . . . . . . . . . 141
  ATC and Varian . . . . . . . . . . . . . . . . . . . . . . . . . . 141
  CO Meter . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 141
  Air Generators . . . . . . . . . . . . . . . . . . . . . . . . . . 141
  General . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 142

Early Morning Checkout . . . . . . . . . . . . . . . . . . . . . . . . 144

Run Pack-Up Checklist . . . . . . . . . . . . . . . . . . . . . . . . . 146

B HC Tank Calibration Source Certification 147

C Official Calibration Sources 168

D CALANA Plots and Analysis Reports 178

# Tables

1. Methanol Target Experiments . . . . 3
2. NO Tank Calibration Sources . . . . 22
3. HC Tank and Liquid Calibration Sources . . . . 22
4. OCS from Injections in Chamber . . . . 24
5. Species ID Numbers and Properties . . . . 26
6. Comparison of Primary NO Calibration Sources . . . . 29
7. Intercomparisons Among Sources . . . . 39
8. Comparison of Primary HC Calibration Sources . . . . 39
9. Processing System for Instrument Auto-Calibration Data . . . . 49
10. CALSUM Example . . . . 50
11. $NO_X$ and $O_3$ Calibrations for 1984 . . . . 56
12. Processing System for Instrument Auto-Calibration Data . . . . 61
13. Summary of CALANA statistics . . . . 67
14. Record Description for RUNENTRY Database System. . . . . 81
15. RUNENTRY Processing Summary for September 14, 1981 . . . . 82
16. Processing System for DVM Data . . . . 93
17. Processing System for Instrument Data . . . . 97
18. Documentation Steps . . . . 100
19. Final Segmented File Production Steps . . . . 106
20. Example Segmented Data File . . . . 110
21. VAX/VMS ANSI VOL1 Label . . . . 120
22. First File Header Label (HDR1) Fields . . . . 121
23. Second File Header Label (HDR2) Fields . . . . 122
24. Third File Header Label (HDR3) Fields . . . . 123

# Figures

1. Comparison of Primary NO Calibration Sources . . . . . . . . . . . . . . . . . 28
2. $NO_X$ and $O_3$ Cal Processing Flowchart . . . . . . . . . . . . . . . . . 32
3. LOTUS Spreadsheet for Manual Cal Processing . . . . . . . . . . . . . . . . . 33
4. LOTUS Analysis Spreadsheet of Manual Cal . . . . . . . . . . . . . . . . . 35
5. LOTUS Analysis Spreadsheet Manual Cal Plots . . . . . . . . . . . . . . . . . 37
6. Official Calibration Source Form . . . . . . . . . . . . . . . . . 45
7. Cal Pick Instruction Form . . . . . . . . . . . . . . . . . 47
8. AUTOCAL Processing Flowchart . . . . . . . . . . . . . . . . . 55
9. HC Autocal Processing Flowchart . . . . . . . . . . . . . . . . . 60
10. CALANA Example Figures . . . . . . . . . . . . . . . . . 64
11. Calextr Examples . . . . . . . . . . . . . . . . . 69
12. Runsheet . . . . . . . . . . . . . . . . . 74
13. Instrument Checklist Form . . . . . . . . . . . . . . . . . 75
14. Run Folder Inventory Checksheet Form . . . . . . . . . . . . . . . . . 76
15. Data Processing Instruction Form . . . . . . . . . . . . . . . . . 78
16. Runentry Welcome and Main Menu Screens . . . . . . . . . . . . . . . . . 83
17. RUNENTRY Date and Display Selection Screens . . . . . . . . . . . . . . . . . 84
18. RUNENTRY General, Documentation, and File Status Screens . . . . . . . . . . . . . . . . . 85
19. RUNENTRY DVM and Picked Instrument Status Screens . . . . . . . . . . . . . . . . . 86
20. PC Report Example . . . . . . . . . . . . . . . . . 87
21. DVM Processing Flowchart (Computers and Files) . . . . . . . . . . . . . . . . . 92
22. Instrument Processing Flowchart (Computers and Files) . . . . . . . . . . . . . . . . . 96
23. Documentation Processing Flowchart (Computers and Files) . . . . . . . . . . . . . . . . . 101
24. Basic Layout of a VAX/VMS ANSI Labeled Volume . . . . . . . . . . . . . . . . . 114
25. Single File/Single Volume Configuration . . . . . . . . . . . . . . . . . 115
26. Multifile/Multivolume Configuration . . . . . . . . . . . . . . . . . 116
27. VAX/VMS ANSI VOL1 Label Format . . . . . . . . . . . . . . . . . 116
28. HDR1 Label Format . . . . . . . . . . . . . . . . . 117
29. HDR2 Label Format . . . . . . . . . . . . . . . . . 118
30. Blocked Fixed-Length Records . . . . . . . . . . . . . . . . . 119
31. Variable-Length Records . . . . . . . . . . . . . . . . . 119

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# 1

# Overall QA Steps

## Introduction

There are a number of general activities that contribute to overall quality in the experimental data. These include:

- having clearly established experimental program goals;
- establishing facilities and analytical support requirements;
- planning activities for experimental and quality assurance programs required to achieve goals;
- reviewing and scheduling activities;
- maintaining basic Research Site Facility;
- using checklists;
- using preventative maintenance;
- performing special test experiments routinely.

Each of these will be discussed further.

## Clearly Established Goals

The most basic part of a QA program is to assure that efforts are properly designed and directed towards clearly defined goals. This assures that the data obtained will satisfy the needs of the program. The approach and design of the experimental program and the selection of experiments are as important as the accuracy and precision aspects of the final data. A range of experiments conducted with appropriate chemical conditions must be identified. Minimum data requirements must be determined beforehand to assure that the results will be useful to achieve the program goals.

The experimental conditions of interest must be identified and prioritized. The number of experiments to be performed are decided based upon program goals, approach, design and resources.

Once an experimental program is designed, a table of Prioritized Target Conditions can be made to guide the experimental program. An example table is shown in Table 1.

Specific experimental conditions of species (and sources) and amounts (chamber concentrations; milligrams of solids, microliters of liquids, or seconds at specific flowrates of gases) are calculated by the project coordinator and recorded on the Run Sheet used to conduct the experiment to assure that the proper experiment is conducted. This form will be discussed further in the chapter entitled "Experimental Data Processing".

## Facilities and Analytical Support Requirements

The facilities and analytical support requirements must be identified. Special modifications or implementation of new analytical methods consume resources. These activities could potentially hinder the attainment of the project goals if problems are encountered. Facilities and analytical capabilities are described in two Appendices attached to each Final Report.

## Planning of Activities

### Calibrations

All instruments must be calibrated frequently to assure accuracy and to determine precision. Along with scheduling the experimental program, scheduling of calibrations are required to assure that the data can be processed with minimal uncertainty. Calibration procedures will be discussed in the next chapter.

### Characterization Runs

Several types of smog chamber experiments are generally conducted to characterize aspects which can effect interpretation of experimental results and aid modelers.

## Table 1. Methanol Fuel Reactivity Experiments

(All experiments have 0.35 ppm $NO_x$)

| Num | TYPE | REACTANTS<br>First Side | REACTANTS<br>Second Side | PURPOSE |
|---|---|---|---|---|
| 1 | Reduction, 33%<br>mid-ratio | 3.00 ppmC SynAuto | 2.00 ppmC SynAuto | To determine the effect of 33% reduction in HC in an *auto-exhaust*-like environment at a typical HC-to-$NO_x$ ratio. Expect 30% reduction in ozone maximum. |
| 2 | Substitution<br>mid-ratio<br>normal HCHO | 3.00 ppmC SynAuto | 2.00 ppmC SynAuto<br>0.89 ppmC MeOH<br>0.01 ppmC $MeNO_2$<br>0.10 ppmC HCHO | To determine the reactivity of the most likely methanol fuel exhaust in an *auto-exhaust*-like environment at a typical HC-to-$NO_x$ ratio. Expect 20% reduction in ozone maximum. |
| 3 | Substitution<br>mid-ratio<br>low HCHO | 3.00 ppmC SynAuto | 2.00 ppmC SynAuto<br>0.99 ppmC MeOH<br>0.01 ppmC $MeNO_2$ | To determine the reactivity of the lowest reactivity methanol fuel exhaust in an *auto-exhaust*-like environment at a typical HC-to-$NO_x$ ratio. Expect 30% reduction in ozone maximum. |
| 4 | Substitution<br>mid-ratio<br>high HCHO | 3.00 ppmC SynAuto | 2.00 ppmC SynAuto<br>0.79 ppmC MeOH<br>0.01 ppmC $MeNO_2$<br>0.20 ppmC HCHO | To determine the reactivity of a highly reactive methanol fuel exhaust in an *auto-exhaust*-like environment at a typical HC-to-$NO_x$ ratio. Expect less than 10% reduction in ozone maximum. |
| 5 | Reduction, 33%<br>low-ratio | 1.000 ppmC SynAuto | 0.666 ppmC SynAuto | To determine the effect of 33% reduction of HC in an *auto-exhaust*-like environment at a *low* HC-to-$NO_x$ ratio. Expect a large reduction in ozone maximum. |
| 6 | Substitution<br>low-ratio<br>normal HCHO | 1.000 ppmC SynAuto | 0.666 ppmC SynAuto<br>0.300 ppmC MeOH<br>0.003 ppmC $MeNO_2$<br>0.030 ppmC HCHO | To determine the reactivity of the most likely methanol fuel exhaust in an *auto-exhaust*-like environment at a *low* HC-to-$NO_x$ ratio. Expect a large reduction in ozone maximum. |

## Table 1, cont'd. Methanol Fuel Reactivity Experiments

(All experiments have 0.35 ppm $NO_x$)

| Num | TYPE | REACTANTS First Side | REACTANTS Second Side | PURPOSE |
|---|---|---|---|---|
| 7 | Reduction, 33%<br>mid-ratio | 3.00 ppmC SynUrban | 2.00 ppmC SynUrban | To determine the effect of 33% reduction in HC in an *urban*-like environment at a typical HC-to-$NO_x$ ratio. Expect 30% reduction in ozone maximum. |
| 8 | Substitution<br>mid-ratio<br>normal HCHO | 3.00 ppmC SynUrban | 2.00 ppmC SynUrban<br>0.89 ppmC MeOH<br>0.01 ppmC $MeNO_2$<br>0.10 ppmC HCHO | To determine the reactivity of the most likely methanol fuel exhaust in an *urban*-like environment at a typical HC-to-$NO_x$ ratio. Expect 20% reduction in ozone maximum. |
| 9 | Substitution<br>mid-ratio<br>high HCHO | 3.00 ppmC SynUrban | 2.00 ppmC SynUrban<br>0.79 ppmC MeOH<br>0.01 ppmC $MeNO_2$<br>0.20 ppmC HCHO | To determine the reactivity of a highly reactive methanol fuel exhaust in an *urban*-like environment at a typical HC-to-$NO_x$ ratio. Expect 10% reduction in ozone maximum. |
| 10 | Substitution<br>low-ratio<br>normal HCHO | 1.000 ppmC SynUrban | 0.666 ppmC SynUrban<br>0.300 ppmC MeOH<br>0.003 ppmC $MeNO_2$<br>0.030 ppmC HCHO | To determine the reactivity of a typically reactive methanol fuel exhaust in an *urban*-like environment at a low HC-to-$NO_x$ ratio. Expect large reduction in ozone maximum. |
| 11 | Substitution<br>high-ratio<br>normal HCHO | 6.00 ppmC SynAuto | 4.00 ppmC SynAuto<br>1.78 ppmC MeOH<br>0.02 ppmC $MeNO_2$<br>0.20 ppmC HCHO | To determine the reactivity of the most likely methanol fuel exhaust in an *auto-exhaust*-like environment at a high HC-to-$NO_x$ ratio. Expect 20% reduction in ozone maximum. |
| 12 | Chemistry | 1.00 ppmC HCHO | 1.00 ppmC HCHO<br>1.00 ppmC MeOH | To illustrate the chemistry of methanol in a highly reactive environment. |

These are performed throughout the programs. A discussion of chamber background reactivity was given in Jeffries and Sexton[12].

### Special Mixtures

The experiments often utilize synthetic mixtures. These mixtures require extensive experimental support. For example, previous experiments may compare the reactivity of these mixtures with real auto exhaust or with other synthetic mixtures which are further compared with simpler photochemical systems. This previous experimental experience is an additional QA step which assures reference to well-studied photochemical systems.

These mixtures are either ordered from scientific gas suppliers or are mixed and prepared on site. In either case, the resulting mixtures are compared with NBS-traceable calibration sources.

### Special Techniques

Some project goals require the development of special techniques such as the production of a particular dilution rate profile or the use of highly labile compounds such as methyl nitrite. To use methyl nitrite requires that the synthesis, storage and use (injection into chamber) techniques be developed and implemented.

## Reviewing and Scheduling Methods

To maximize the quality of program results, reviewing and careful scheduling are needed throughout the program. Important considerations are the priority of the experiments, status of the smog chamber site facilities, weather, and previous experimental results. Inherent in this process is a continuous review of experimental results to assure that target conditions are being attained and experimental conditions were satisfactory.

### Priority of Runs

The results of experiments are affected by the initial concentration conditions, even for the same composition of ozone precursors. For most studies, several experiments are desired. Higher priorities are assigned to those experiments which will yield the most information for the more average conditions. Later experiments are used to establish the range of conditions or to establish more basic results to assist in interpretation.

### Use of NOAA Weather Radio

Outdoor Smog Chambers are subjected to real weather situations. This leads to difficulties in scheduling runs. To provide up-to-the-minute information needed to schedule runs, we use a weather radio to receive the airport NOAA weather radio station. Weather reports are updated every hour and forecasts are made every 3 minutes. The most desirable conditions are clear, sunny, dry and warm.

When clear weather is forecast, the site operator is contacted by telephone. He gives a status report of the site facilities and instrumentation. The next highest priority experiment which can be conducted considering the current status of the facilities is then scheduled.

When cloudy weather is forecast ("partly cloudy") with a low probability of rain, a characterization experiment is scheduled unless a set of calibrations are needed and the long range forecast is for good weather.

When rainy or "mostly cloudy" weather is forecast, a "CAL DAY" is scheduled.

### Feedback Scheduling

Experimental results are reviewed frequently. Experiments are repeated or new experiments are designed and scheduled depending on the conditions or outcome of experiments already conducted.

## Site Operation

A great deal of QA occurs in the routine operation of the smog chamber site. Procedures more basic than calibrations are required to assure useful and complete data. The laboratory itself must be maintained. Adequate supplies must be in place, all documentation must be complete, instruments must be in good operating order, support equipment must be checked-out, and the chamber must be cleaned and leak-checked.

### Lab Air Conditioner

The laboratory air conditioner maintains a consistent environment needed for the operation of instruments and computers in the typical 95°F, high humidity, summer conditions in North Carolina. Lab temperature is monitored continuously by the computer data acquisition system and is reported in the final distributed experimental results segmented data file. The lab temperature is maintained at 75°F. The air conditioner is checked at the beginning of every run season by a professional service. The filter is changed every three weeks during most of the season and every two weeks during the warmest part of the season.

### Smog Chamber

The smog chamber itself requires routine maintenance. It is frequently checked for holes and leaks, which are repaired. Occasionally insects find their way into the chambers and must be removed. The floor is swept and sponged with distilled water when needed. The automated venting doors and air drying ductwork is checked daily. Leaks are often discovered by analysis (least-squares exponential fit: see section on computer programs below) of the inert tracer data collected during every run on both sides of the dual chamber.

### Chamber Sampling Manifold

The sampling manifold is routinely checked for breaks. It is warmed with electric heat tapes the entire length from the chamber to the fans inside the laboratory. Minor leaks can be discovered by analysis of the inert tracer data collected during every run on both sides of the dual chamber. The manifold is checked daily for breaks, inoperating heating lines by touch, and by appearance of condensation (warm chamber air into a cooler laboratory).

### Chamber AC Drying System

An automated chamber air drying system in place under the chamber is used before experiments to prevent condensation which might form during the cool morning hours after venting the chambers. A Freon check and general maintenance checkout is performed at the beginning of every run season. Testing is performed early in the season to measure the dewpoint depression capability. Routine monitoring of daily performance (for each experiment) is the most common QA procedure. Dewpoint is continuously monitored. Condensation is checked by the morning operator.

### Ethylene Convertor

The ozone monitor utilizes ethylene. The excess is routed through a heated convertor which oxidizes it. Untreated excess ethylene can be a severe contamination problem. To check for leaks in the ethylene treatment system, two GC-FID systems (Carles 1 and 2) monitor for this possible contamination in background chamber air analyses before every experiment.

### Mass Balance

A high precision Mettler balance is used for weighing chemicals used for reagents and paraformaldehyde used for injection of formaldehyde into the chamber.

### Supplies

An inventory is performed at the beginning of every run season to determine supplies which must be ordered long in advance of the run season. Special mixtures of HC and other precursors must also be ordered. More common supplies are tracked and stocked routinely. During the run season, the use of expendable supplies is carefully monitored and reordered when necessary.

## Check Lists

Many details must be checked to assure that a smog chamber experiment will be successful. Several checklists are used before, during, and after experiments.

### Setup Checkout Lists

To make sure that things are ready for an experiment the next day, a setup checkout list is used. All supplies (gases, *etc.*), computer and instrument switch settings, and injection gases are checked; syringes and liquid chemicals are set out; the run sheet is filled out; venting is checked; the manifold is checked for leaks, *etc*. This checklist is shown in Appendix A.

### Operator Checkout List

For the early morning operator responsible for initiating the experiment, another checklist is used. This is somewhat redundant to the setup list to check extremely important details that might have been overlooked by the setup operator. In addition, check items include details about proper operation of instruments, manifold, and chamber, injections of chemical precursors, and recording documentation about details of experiment. This list is also shown in Appendix A.

### Run Checkout List

Another checkout list is used by site personnel that arrive at mid-morning. Check items include checking on status of instruments, stripchart recorders, computer, chamber, *etc.* to assure successful continuation of the experiment and data acquisition. This list is also given in Appendix A.

### Run Packup List

This list is primarily an inventory checklist to insure that all data is properly packed up, documented, and returned to the School of Public Health data processing office. This list is included in Appendix A.

## Preventative Maintenance

To assure proper operation of all instruments, the smog chamber, support facilities, instrument stability (reflected in "cal factor variation"), and maximum "up-time," preventative maintenance is routinely performed.

## Characterization Experiments

As mentioned above, characterization experiments are performed routinely. These experiments are used by modelers to determine the importance of chamber artifact processes. Background, reactivity, surface processes (such as off-gasing of $NO_x$, HCHO), decay of $O_3$ and $NO_x$ are of primary interest. Previous experiments conducted over several years have been studied to characterize these and other aspects of chamber behavior. Benchmark experiments are also routinely performed. These include propylene and $NO_x$ experiments.

### Types of Characterization Experiments

*Background*

This experiment shows how much $O_3$ is formed when no chemical precursors are injected into the chamber except for the rural air used in venting and any material which may remain on the chamber walls after venting.

*O3 Decay*

$O_3$ is injected into otherwise clean air and allowed to decay. The rate is determined. This experiment is usually performed at night. Some modelers include this decay process although the rate is very low.

*NO Oxidation, Daytime*

NO is injected into clean chamber air (nothing else injected) to detect sources of radicals. The rate of oxidation is observed. The magnitude of and types chamber radical sources required to achieve the observed rate can be estimated by modeling. To modify the test, CO can be added to one side to help determine the type of radical source. The CO changes the balance of $HO^\cdot$ and $HO_2^\cdot$ radicals without adding any radicals to the system itself.

### *NO Decay, Nighttime*

This experiment is conducted like the one described above except that no sunlight is involved.

### *Acetaldehyde and CO*

Matched injections of acetaldehyde (usually 1 ppmC) are made into each chamber. One side has CO injected (usually 50 ppm). This experiment forms PAN which can aid in detecting any wall $NO_x$ off-gasses. The CO changes the balance of $HO^\cdot$ and $HO_2^\cdot$ radicals without adding any radicals to the system itself.

### *Formaldehyde and CO*

Matched injections of formaldehyde are made into each chamber. One side has CO injected (usually 50 ppm). Formaldehyde photolyzes to produce $HO_2^\cdot$ and CO. Without injected $NO_x$, only the background $NO_x$ in the rural air or from the chamber walls can participate in this system. Any HO produced can react with formaldehyde or with the additional CO added to one side. The CO changes the balance of $HO^\cdot$ and $HO_2^\cdot$ radicals without adding any radicals to the system itself.

### *Propylene and NOx*

Matched conditions of propylene and $NO_x$ have been used for years as a benchmarking experiment. Experience has shown that experiments conducted on the same day a year apart can be duplicated if the sunlight quality is good. Demonstrating matched results from the two chambers is another reason for conducting matched condition experiments.

## Frequency

These experiments should be conducted routinely. However, they are not conducted as frequently when the program falls behind schedule because of poor weather. These experiments have been studied and the range of magnitude of these chamber processes is well known.

# 2

# System Components

This section lists and describes the system components. Major types of tasks and responsibilities have been organized and assigned to different people. Computers, instruments and other hardware are used to generate and process data. Many computer programs (software) are used. Policies and procedures have been developed to assure proper and consistent treatment of the data. Databases have been created to organize and to aid in retrieving and processing the large amounts of calibration data.

## Location of Work

The research work occurs in two different locations. The experiments are conducted at the Smog Chamber Site located in a rural area with relatively clean background air, and the data is processed on the University campus.

### Experimental Site

The site is located in Chatham County, North Carolina, approximately 32 kilometers from the University of North Carolina at Chapel Hill, and approximately 10 kilometers from the small town of Pittsboro. Chatham County is one of the most rural, least industralized counties in North Carolina and is heavily wooded. The background concentrations of $NO_x$ and NMHC are usually less than 5 ppbC and less than 80 ppbC. More importantly, the air exhibits very low reactivity in the chamber.

## Data Processing Location

The data are processed in the School of Public Health on the campus of UNC, where all computers and data processing facilities are easily accessible.

# Personnel

A number of people with different tasks contribute to the process of conducting smog chamber experiments and processing the results. The names and roles of these people are listed below.

### Advisory Group, AG

An advisory group, consisting of the principal investigator, the co-principal investigator, the project coordinator, and the administrative research assistant meet frequently to review the progress of each project.

### Administrative Research Assistant, AA

The administrative research assistant is responsible for logging the experiments and calibrations, ordering supplies, and managing the budget.

### Project Coordinator, PC

The project coordinator oversees the experimental program and the processing of the data.

### Site Operator, SO

Site operators are responsible for maintenance, calibration, and operation of the research site. They work closely with the PC to determine which experiments should be conducted next or if time should be scheduled for calibration or maintenance.

### Peak Picker, PP

The "peak pickers" process most of the data under the guidance of the PC.

### Computer Technician, CT

The computer technicians are responsible for unpacking the data from the smog chamber data acquisition system and for making tapes of segmented data files and a backup of all data processing files.

## Computers Used

Several computers are used in the program. They help conduct experiments, process data, plot data, analyze results, and aid in writing.

### DEC PDP-11/40

The DEC PDP-11/40 is used to control the experiments and perform the data acquisition for much of the data. This computer writes data to 8 inch flexible diskettes for transfer to the data processing office.

### DEC LSI-11/23

Two DEC LSI-11/23 computers are used to process most of the experimental and calibration data. Most programs are written in PASCAL. A major component is the DIGITIZER which permits rapid and accurate conversion of stripchart data to computer data files. Each computer has at least one 8 inch floppy drive and a 10 Mb hard disk. These computers can communicate to the IBM PC and to the DEC VAX-11/780.

### IBM PC

The IBM PC is used with LOTUS 123 to implement many spreadsheets and databases discussed throughout this report. It is also used for word processing. Some PASCAL programs are also used. The IBM PC uses 5 1/4 inch floppies and can "upload" and "download" data from the DEC VAX-11/780.

### DEC VAX-11/780

A DEC VAX-11/780 mainframe computer is used to maintain several large databases discussed in this report. The VAX system also makes plots and prints reports using a large, high resolution laser printer. Modeling input decks are set up and submitted from the VAX to be run on the university's IBM 4381 mainframe computer. "Printouts" and "punched" output are returned to the VAX as standard ASCII files. The VAX can also read and write to 8 inch floppies and industry standard magnetic tape.

# Computer Programs Used

## Description of General Purpose Programs

### *LOTUS 123*

LOTUS 123 is an electronic spreadsheet, database, and graphic program that runs on the IBM PC. The spreadsheet in 123 has 256 columns and 2096 rows; each column can be a different width and each cell can hold a text label, a numerical value, or a formula that includes references to other cells. When new data is entered into cells, the program automatically updates the values of all the formulas. Ranges of cells can be selected to be graphed. Graphs include line, bar, and pie; up to 6 lines can be plotted on a graph. In addition, the spreadsheet contents can be treated like a database table in which the rows are records and the columns are fields in the record. Records can be selected, deleted, copied, and sorted to an output location on the spreadsheet. The whole spreadsheet or selected parts of the spreadsheet can be printed to a printer or file. Data can also be 'imported' from other programs or files.

### *DATATRIEVE*

DATATRIEVE is a data base query, update, and report writing system running on the VAX-11. DATATRIEVE is used to maintain calibration and data processing status databases and serves a tool to coordinate effort among the PC, PP, and CT. In DATATRIEVE, the PC can ask the system to print a list of all runs that had all instrument data "picked" but did not have calibration factors determined for those instruments. From this list, the PC determines which calibration factors must be produced to complete the processing of the runs. Typical run tracking data bases grow to be 500,000 characters during a run processing season. The total size of data managed by DATATRIEVE is more than 20 million characters.

## Description of Specific Programs

*UNPACK* converts packed binary DVM data from the chamber site's DA system to ASCII format ("U files").

*FASTDV* produces temporary ("P" file) files of raw DVM data for making plots for preliminary QA procedures, and strips $NO_x$ and $O_3$ calibration data from DVM data file.

*DIGPIK* allows the digitizer to be used to convert experimental peak height data for all species for a given instrument and writes data to ("P" file) files on LSI11/23.

It also is used to digitize calibration data and produce calibration response ("R") files.

*PLOPIC* plots raw ("P" file) experimental data from both DVM or stripcharts.

*ACALAV* automatically produces average $NO_x$ and $O_3$ instrument calibration data for zeros and spans stripped from the DVM data with FASTDV.

*CALFAC* calculates calibration factors from digitized calibration data and the official calibration source file.

*CALLOK* lists and plots calibration data for a given instrument and species combination.

*CALANA* performs statistical analysis on calibration data for any combination of instrument and species.

*DVMFIX* applies calibration factors to DVM ("U" file) data and outputs concentration and physical measurement ("G") files.

*CALCON* applies calibration factors to digitized ("P" file) data from stripcharts and outputs concentration ("C" files).

*PLOCON* plots concentration ("C" file) experimental data from stripcharts.

*HCANAL* reads time/concentration data files of HC data and computes composition analysis.

*CSTAR* reads tracer data files and computes chamber dilution rate by fitting with exponential least-squares method.

## Description of Data File Formats and Contents

### "U" file

The primary data file originating from the Data Acquisition system is "U"npacked after transport from the chamber site to the data processing office. This file contains "raw" data from the $NO_x$ and $O_3$ monitors, chamber, ambient and laboratory temperature, total solar and ultraviolet light, and dewpoint monitors. The data is taken every minute alternating between the two sides. Calibration data from automatic calibrations of the $NO_x$ and $O_3$ monitors is also contained in this file.

## "G" file

The final data file processed from the primary "U" file is referred to as the "G"as Chamber file. This file contains corrected (adjusted with calibration factors) data. The final data is for four minute intervals alternating between the two sides.

The file is comprised of two parts: documentation and data. The documentation identifies the experiment. Next information pertaining to the processing of the data is given:

- source of calibration factors;
- data last processed;
- explanation of data identifiers (labels);
- explanation of units;
- explanation of data alteration.

Finally the actual calibration factors are listed. Calibration factors are specified for the beginning and ending of periods of valid data.

The data are preceded by a "header" card identifying the columns of data. Data are listed in the same order as the header card. An example of this type of file is shown in Chapter 6.

## "P" files

The data files of "P"icked data from other individual instruments which are not connected to the Data Acquisition System are produced and processed separately with more manual effort (*e.g.*measuring peak heights from gas chromatographs). This file is comprised of two parts: documentation and data. The documentation indicates:

- the source of the data;
- the data processor ("peakpicker");
- attenuation;
- units;
- species identification.

The data follows with one data point per line: the format allows for easy editing and correction during processing.

### "C" files

These are the files of final corrected "C"oncentration data processed from the "P" files. The format of these files are identical to the data portion of the "G" files. An example of this type of file is shown in Chapter 6.

### "K" files

For every "C" file there is a matching "K" file containing documentation pertaining to the source and processing of the data. In addition to the documentation originally in the "P" file is the maximum amplitude and concentration of each species in the file and the calibration factor (and source) used in processing the data. An example of this type of file is shown in Chapter 6.

### "R" files

Calibration "R"esponse data to official calibration sources other than from the $NO_x$ and $O_3$ monitors are stored in these files, which are produced from the same program which produces the "P" files (DIGPIK). They have very similar format and documentation but also include the OCS identification number.

### "Q" files

The resulting calibration factors from comparing the "R" files to the Official Calibration Sources are stored in the "Q" files along with all associated documentation from the "R" file. This file also contains DATATRIEVE commands which will store the data in the calibration DATATRIEVE database HCCAL.

### "A" files

Calibration response data from the "A"utomatic calibrations of the $NO_x$ and $O_3$ monitors are produced with FASTDV from the data stored in the "U" file.

### "E" files

The "A" files often contain data which represent a transition reading between the chamber air and the calibration source. This unwanted data is "E"dited from the file.

## ACDTR.COM file

The "E" files are processed (averaged) to a single value with a program called ACALAV which is output to a file called ACDTR.COM which also contains DATATRIEVE commands to store the data in the DATATRIEVE database AUTOCAL.

## Description of Databases

Several databases are used in processing the data and calibration data. The following are created with DATATRIEVE on the VAX-11/780. These are described in more detail in Chapter 3.

*RUNENTRY* is the primary database identifying the experiment and tracking the processing of the data from each instrument used.

*CAL_ENTRY* is the database for tracking the calibration data processing.

*CAL_SOURCES* is the database of the "O"fficial "C"alibration "S"ources OCS) including all supporting information and corresponding identification number.

*HC_CAL* is the database of the final processed calibration factors resulting from calibrations performed on the analytical instruments producing data which is not collected from the Data Acquisition System.

*AUTO_CAL* is the database of the calibration data from "auto"matically performed calibrations of the $NO_x$ and $O_3$ monitors.

*RUN_CAL_USED* is the database of the calibration factors actually used in processing the manually processed ("P" file) data.

*SPECIES* is the database of official species names and corresponding identication numbers used in data processing to assure consistency and proper spelling and identification.

## Description of Database Procedures

### List of all DTR Procedures by Name and Function

Various procedures are used with the DATATRIEVE databases to assist in accessing and using the data and producing reports or files to be used by other data processing computer programs.

*PPREPORTS* is a VAX command procedure which creates a task report for Peak Pickers (data processors running DIGPIK using DATATRIEVE and the RUNENTRY data base. The report lists each data processing step presently needing PP action, such as instrument stripcharts needing to be digitized and plotted.

*PCREPORTS* is a VAX command procedure which creates a task report for Project Coordinators using DATATRIEVE and the RUNENTRY data base. The report lists each data processing step presently needing PC action, such as various QA steps.

*CTREPORTS* is a VAX command procedure which creates a task report for Computer Technicians using DATATRIEVE and the RUNENTRY data base. The report lists each data processing step presently needing CT action, such as moving data to the VAX or vice versa.

*PRINT_SPECIES* prints a list of the official species names and corresponding identification number.

*PRINT_CAL_SOURCES* prints a list of the Official Calibration Sources including name, serial number, source date, validation date and personnel, manufacturers and the validated concentrations.

*PRINT_OCS_FILE_FOR_LSI* produces a file of the official calibration sources to be used by another program (CALFAC) used to calculate calibration factors from the calibration response data.

*PRINT_CALS_AND_FACTORS* calculates and produces a report of the calibration factors calculated from the automatic calibration data from the $NO_x$ and $O_3$ monitors from the AUTO_CAL database.

*PRINT_HC_CAL_FACTORS* produces a report of the calibration data for all the other instruments other than $NO_x$ and $O_3$monitors from the HC_CAL database.

*PRINT_RUN_CAL_USED* - produces a report of the calibration factors used by instrument, species, and date from the RUN_CAL_USED database.

*PRINT_CALENTRY_SUM_ON_FILE* produces a summary report of all calibration data processing steps completed by date, by instrument from the CAL_ENTRY database.

### Worksheets/Databases

Several worksheets implemented with the LOTUS 123 software on the IBM PC are used. These are backed-up on 5.25 inch floppy diskettes. Each of these will be discussed in detail in Chapter 3.

OCSICyy - Injections into the smog chamber are used as calibration sources. This worksheet/database calculates the chamber concentration from the amount injected, the chamber temperature, the ideal gas law, and compound physical data from a lookup table in the worksheet. A different worksheet is maintained for each year (yy).

CAL - All hydrocarbon calibration sources are compared and "validated" in this worksheet/database. It is listed in Appendix B.

MANmmddyy - "Man"ually performed gas phase titration calibrations for the $NO_x$ and $O_3$ monitors are processed in this worksheet. One worksheet is produced for each calibration identified by date (month, day, year).

MANCALyy - The calibration factors resulting from the MANmmddyy worksheets is analyzed in this worksheet.

# 3

# Calibration

## Approach

All instruments are calibrated at a minimum of two reference levels: a "zero" and a "span" point. The latter is generally near the expected maximum concentration in the experiments. "Zero" air samples are obtained by sampling from a zero air generator or by sampling from a filter specific for the species being monitored. "Span" values are generated from several sources that will be described below. During the programs, different "span" levels are used. These different levels assure that linearity can be checked in final QA procedures, to be discussed in later sections. Several different calibration standard sources, including NBS traceable sources and sources from outside groups, are utilized and compared. Calibrations for most instruments are performed immediately before an experiment. $NO_x$ and $O_3$ monitors are calibrated twice daily. These calibration data are used to adjust the data collected in final data processing steps after the calibration data itself has been processed and reviewed in the context of the entire calibration database for the season.

## NBS-Traceable Sources

### NO and O3 Sources

Two techniques are used to calibrate the chemiluminescent $NO_x$ and $O_3$ monitors. The primary technique is the EPA gas-phase titration method[3] which utilizes a high concentration NO source (NBS-traceable) as the primary standard. Comparison of this primary source with other sources is performed regularly. In one recent study, three of these high concentration sources were compared and found to agree within a few percent of each other. Low concentration sources of NO and $O_3$ are also used to perform span checks more frequently and automatically (AUTOCAL source). Low concentration (<1 ppm) pressurized gas cylinders are used for NO sources, and a generator built into the $O_3$ monitor is used for the $O_3$ AUTOCAL source. These are calibrated and used as transfer standards. Table 2 lists the calibration sources used for $NO_x$.

**Table 2. NO Tank Calibration Sources**

| Name | Manuf. | Manf. ID | UNC ID | OCS ID |
|---|---|---|---|---|
| NO 46.0 ppm | Matheson | SX-13759 | UNCAB2113 | 94 |
| NO 52.4 ppm | Airco | 1122590 | UNCBC9045 | 169 |
| NO 52.6 ppm | Scott | BAL177 | UNCAB0348 | 170 |
| NO 0.823 ppm |  | CC-15860 |  | 4 |
| NO 0.288 ppm |  |  |  | 171 |
| NO 0.665 ppm | Airco | CC-15780 | UNCAB2478 | 172 |

The OCS ID heading will be explained below.

## Hydrocarbon Sources

Commercially prepared NBS traceable calibration sources are also used for hydrocarbons. Five different tanks purchased by UNC were used. In addition, two other tanks were borrowed from the Research Triangle Institute (RTI) who is involved in a multiyear intercomparison of commercial hydrocarbon calibration sources. A low concentration tank prepared from diluting a small portion of one of the commercially prepared high concentration tanks was calibrated as a transfer standard for automatic calibration. These calibration sources are listed in Table 3. Another source of hydrocarbon standards was prepared in the chambers by injecting liquid hydrocarbons. These are listed in Table 4. The identities and properties of the species calibrated this way are given in Table 5. All sources were compared and results are described below.

## Table 3. HC Tank and Liquid Calibration Sources

| | | | | |
|---|---|---|---|---|
| NEW AIRCO | Airco | X-3362 | UNCAB2467 | 112 |
| LOW MW (HC) | Scott | AAL11557 | UNCAB2136 | 109 |
| LOW MW (LC) | UNC | NA | NA | 111 |
| HIGH MW | Scott | AAL11551 | UNCAB2139 | 108 |
| RTI- ethylene | | 2H | | 167 |
| RTI- propylene | | 3A | | 168 |
| 82HCCALMIX | | XA-1336 | | 1 |
| NEWSCOTTCALTANK | | | | 110 |
| LIQ STD 8/14 | | NA | | 123 |

### Transfer Standards Created from Primary Sources

For $NO_x$, $O_3$, and hydrocarbons, several sources traceable to NBS are used. These are high concentration tanks for stability and accuracy which require dilution or instrument attenuation adjustment when used. Accurate liquid injections into the smog chamber are also considered as primary standards. Several low concentration NO tanks were purchased as a source for automatic calibrations ("AUTOCAL" sources). A low concentration HC tank was prepared by diluting a portion of the LOW MOLECULAR WEIGHT (high concentration) calibration tank into an empty tank with nitrogen to be used as an AUTOCAL source. AUTOCAL sources do not require a morning operator to be present to change the attenuation settings and are not subject to possible errors from dilution. These calibration sources were intercompared. The RTI tanks were considered absolute because of their extensive comparative analysis history. In the case of the hydrocarbon sources, some judgements resulted in small adjustments to the "validated" concentrations to make all the UNC sources more consistent. The intercomparison procedures result in calibration of the AUTOCAL sources.

## Primary Source Comparison

### NO and O3 Sources

This test is conducted to compare the manufacturers stated analyzed gas concentrations of the NO tanks. Nitrogen oxide tanks are available for use in the EPA Gas Phase Titration method (see description in "Routine $NO_x$ and $O_3$ Calibrations"). Three tanks with NO concentrations of 52.6, 52.4, and 46 ppm (see 2) were diluted with clean air (zero air generator) to concentrations of approximately 0.2, 0.6 and

# Table 4.

OFFICIAL CALIBRATION SOURCES FROM INJECTIONS INTO SMOG CHAMBER

LAST UPDATE: 13-JUN-85

CHAMBER VOLUME 150000 (L) STP VOL: 22.414 (L)

| OCS ID # | OCS NAME | SOURCE DATE | SPEC ID # | C # | DENSITY | MW | UL or G | T F | PURITY | CONC UL | CONC G |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 95 | | 6/25 | 68 | 8 | 0.864 | 106.1 | 283.000 | 70.0 | 100% | 2.9679 | NA |
| 96 | | 6/25 | 55 | 7 | 0.867 | 92.14 | 556.000 | 70.0 | 100% | 5.8955 | NA |
| 97 | | 6/27 | 55 | 7 | 0.867 | 92.14 | 463.000 | 70.0 | 100% | 4.9093 | NA |
| 98 | | 6/26 | 68 | 8 | 0.864 | 106.1 | 283.000 | 71.8 | 100% | 2.9780 | NA |
| 99 | | 6/26 | 71 | 8 | 0.897 | 106.1 | 243.000 | 71.8 | 100% | 2.6530 | NA |
| 100 | | 6/19 | 55 | 7 | 0.867 | 92.14 | 370.500 | 70.0 | 100% | 3.9285 | NA |
| 101 | | 6/19 | 68 | 8 | 0.864 | 106.1 | 282.900 | 70.0 | 100% | 2.9668 | NA |
| 102 | | 7/10 | 139 | 1 | 0.815 | 30.05 | 0.110 | 70.0 | 92% | NA | 0.5421 |
| 103 | | 7/10 | 139 | 1 | 0.815 | 30.05 | 0.210 | 70.0 | 92% | NA | 1.0350 |
| 104 | | 7/11 | 139 | 1 | 0.815 | 30.05 | 0.192 | 70.0 | 92% | NA | 0.9463 |
| 105 | | 7/11 | 139 | 1 | 0.815 | 30.05 | 0.192 | 70.0 | 92% | NA | 0.9463 |
| 106 | | 7/27 | 139 | 1 | 0.815 | 30.05 | 0.192 | 70.0 | 92% | NA | 0.9463 |
| 107 | | 7/27 | 139 | 1 | 0.815 | 30.05 | 0.038 | 70.0 | 92% | NA | 0.1893 |
| 115 | | 7/31 | 139 | 1 | 0.815 | 30.05 | 0.192 | 70.0 | 92% | NA | 0.9463 |
| 116 | | 6/28 | 55 | 7 | 0.867 | 92.14 | 556.000 | 77.3 | 100% | 5.9767 | NA |
| 117 | | 6/28 | 68 | 8 | 0.864 | 106.1 | 283.000 | 77.3 | 100% | 3.0088 | NA |
| 118 | | 7/16 | 40 | 6 | 0.878 | 78.11 | | | 100% | 0.0000 | NA |
| 118 | | 7/16 | 55 | 7 | 0.867 | 92.14 | | | 100% | 0.0000 | NA |
| 118 | | 7/16 | 68 | 8 | 0.864 | 106.1 | | | 100% | 0.0000 | NA |
| 118 | | 7/16 | 71 | 8 | 0.897 | 106.1 | | | 100% | 0.0000 | NA |
| 118 | | 7/16 | 67 | 8 | 0.861 | 106.1 | | | 100% | 0.0000 | NA |
| 118 | | 7/16 | 89 | 8 | 0.906 | 104.1 | | | 100% | 0.0000 | NA |
| 119 | | 7/27 | 82 | 8 | 0.692 | 114.2 | | | 100% | 0.0000 | NA |
| 120 | | 7/27 | 40 | 6 | 0.878 | 78.11 | | | 100% | 0.0000 | NA |
| 123 | | 8/14 | 19 | 5 | 0.626 | 72.15 | 416.000 | 85.0 | 100% | 2.9875 | NA |
| 123 | | 8/14 | 28 | 6 | 0.653 | 86.18 | 420.000 | 85.0 | 100% | 3.1609 | NA |
| 123 | | 8/14 | 42 | 7 | 0.695 | 100.2 | 372.000 | 85.0 | 100% | 2.9897 | NA |
| 123 | | 8/14 | 82 | 8 | 0.692 | 114.2 | 373.000 | 85.0 | 100% | 2.9925 | NA |
| 123 | | 8/14 | 55 | 7 | 0.867 | 92.14 | 274.000 | 85.0 | 100% | 2.9876 | NA |
| 123 | | 8/14 | 68 | 8 | 0.864 | 106.1 | 276.000 | 85.0 | 100% | 2.9765 | NA |
| 123 | | 8/14 | 71 | 8 | 0.897 | 106.1 | 238.000 | 85.0 | 100% | 2.6630 | NA |
| 124 | | 6/27 | 68 | 8 | 0.864 | 106.1 | 188.600 | 70.0 | 100% | 1.9779 | NA |
| 125 | | 7/13 | 139 | 1 | 0.815 | 30.05 | 0.212 | 68.0 | 92% | NA | 1.0384 |
| 126 | | 7/13 | 139 | 1 | 0.815 | 30.05 | 0.212 | 68.0 | 92% | NA | 1.0384 |
| 127 | | | 205 | 1 | 0.791 | 32.04 | 224.000 | 70.4 | 100% | 0.8914 | NA |
| 128 | | | 205 | 1 | 0.791 | 32.04 | 224.000 | 74.0 | 100% | 0.8974 | NA |
| 129 | | | 205 | 1 | 0.791 | 32.04 | 80.100 | 74.0 | 100% | 0.3209 | NA |
| 130 | | | 205 | 1 | 0.791 | 32.04 | 74.700 | 75.5 | 100% | 0.3001 | NA |
| 131 | | | 205 | 1 | 0.791 | 32.04 | 196.700 | 73.0 | 100% | 0.7866 | NA |

## Table 4, cont.

| OCS ID # | OCS NAME | SOURCE DATE | SPEC ID # | C # | DENSITY | MW | UL or G | T F | PURITY | CONC UL | CONC G |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 132 | | | 205 | 1 | 0.791 | 32.04 | 65.500 | 74.5 | 100% | 0.2627 | NA |
| 133 | | 10/7 | 139 | 1 | 0.815 | 30.05 | 0.192 | 54.0 | 92% | NA | 0.9177 |
| 134 | | 10/7 | 139 | 1 | 0.815 | 30.05 | 0.097 | 54.0 | 92% | NA | 0.4636 |
| 135 | | 10/9 | 139 | 1 | 0.815 | 30.05 | 0.192 | 55.0 | 92% | NA | 0.9195 |
| 136 | | 10/9 | 139 | 1 | 0.815 | 30.05 | 0.192 | 55.0 | 92% | NA | 0.9195 |
| 137 | | 10/16 | 139 | 1 | 0.815 | 30.05 | 0.048 | 61.0 | 92% | NA | 0.2325 |
| 138 | | 10/16 | 139 | 1 | 0.815 | 30.05 | 0.096 | 61.0 | 92% | NA | 0.4651 |
| 140 | | 8/25 | 205 | 1 | 0.7914 | 32.04 | 74.000 | 66.2 | 100% | 0.2921 | NA |
| 143 | | 9/1 | 205 | 1 | 0.7914 | 32.04 | 249.000 | 59.0 | 100% | 0.9695 | NA |
| 144 | | 9/3 | 205 | 1 | 0.7914 | 32.04 | 66.900 | 66.7 | 100% | 0.2644 | NA |
| 147 | | 9/17 | 205 | 1 | 0.7914 | 32.04 | 151.000 | 45.0 | 100% | 0.5721 | NA |
| 148 | | 9/25 | 139 | 1 | 0.815 | 30.05 | 0.192 | 62.0 | 92% | NA | 0.9320 |
| 159 | | 9/5 | 139 | 1 | 0.815 | 30.05 | 0.192 | 78.0 | 92% | NA | 0.9606 |
| 162 | | 5/14/85 | 55 | 7 | 0.867 | 92.14 | 92.000 | 86.0 | 100% | 1.0050 | NA |
| 162 | | 5/14/85 | 40 | 6 | 0.878 | 78.11 | 45.000 | 86.0 | 100% | 0.5033 | NA |
| 162 | | 5/14/85 | 68 | 8 | 0.864 | 106.1 | 185.000 | 86.0 | 100% | 1.9988 | NA |
| 162 | | 5/14/85 | 82 | 8 | 0.692 | 114.2 | 240.000 | 86.0 | 100% | 1.9290 | NA |
| 163 | | 5/17/85 | 55 | 7 | 0.867 | 92.14 | 100.000 | 72.0 | 100% | 1.0643 | NA |
| 163 | | 5/17/85 | 40 | 6 | 0.878 | 78.11 | 50.000 | 72.0 | 100% | 0.5449 | NA |
| 163 | | 5/17/85 | 68 | 8 | 0.864 | 106.1 | 200.000 | 72.0 | 100% | 2.1054 | NA |
| 163 | | 5/17/85 | 82 | 8 | 0.692 | 114.2 | 300.000 | 72.0 | 100% | 2.3494 | NA |
| 164 | | 5/20/85 | 139 | 1 | 0.815 | 30.05 | 0.201 | 82.0 | 95% | NA | 1.0461 |
| 165 | | 5/22/85 | 82 | 8 | 0.692 | 114.2 | 100.000 | 80.0 | 100% | 0.7949 | NA |
| 165 | | 5/22/85 | 40 | 6 | 0.878 | 78.11 | 150.000 | 80.0 | 100% | 1.6593 | NA |
| 165 | | 5/22/85 | 55 | 7 | 0.867 | 92.14 | 200.000 | 80.0 | 100% | 2.1607 | NA |
| 165 | | 5/22/85 | 68 | 8 | 0.864 | 106.1 | 400.000 | 80.0 | 100% | 4.2741 | NA |
| 165 | | 5/22/85 | 71 | 8 | 0.897 | 106.1 | 500.000 | 80.0 | 100% | 5.5431 | NA |
| 165 | | 5/22/85 | 78 | 9 | 0.876 | 120.2 | 500.000 | 80.0 | 100% | 5.3791 | NA |
| 166 | | 5/24/85 | 82 | 8 | 0.692 | 114.2 | 100.000 | 65.0 | 100% | 0.7728 | NA |
| 166 | | 5/24/85 | 40 | 6 | 0.878 | 78.11 | 150.000 | 65.0 | 100% | 1.6132 | NA |
| 166 | | 5/24/85 | 55 | 7 | 0.867 | 92.14 | 200.000 | 65.0 | 100% | 2.1006 | NA |
| 166 | | 5/24/85 | 68 | 8 | 0.864 | 106.1 | 400.000 | 65.0 | 100% | 4.1553 | NA |
| 166 | | 5/24/85 | 71 | 8 | 0.897 | 106.1 | 500.000 | 65.0 | 100% | 5.3889 | NA |

**Table 5. Species ID numbers and Properties**

| ID | NAME | # | DENS | MW | PURITY |
|---|---|---|---|---|---|
| 19 | N-PENTANE | 5 | 0.626 | 72.15 | 100% |
| 28 | 2-METHYLP | 6 | 0.653 | 86.18 | 100% |
| 40 | BENZENE | 6 | 0.878 | 78.11 | 100% |
| 42 | 2,3-DIMET | 7 | 0.695 | 100.2 | 100% |
| 55 | TOLUENE | 7 | 0.867 | 92.14 | 100% |
| 60 | N-OXTANE | 8 | 0.703 | 114.2 | 100% |
| 67 | P-XYLENE | 8 | 0.861 | 106.1 | 100% |
| 68 | M-XYLENE | 8 | 0.864 | 106.1 | 100% |
| 71 | O-XYLENE | 8 | 0.897 | 106.1 | 100% |
| 82 | 2,2,4-TRI | 8 | 0.692 | 114.2 | 100% |
| 89 | STYRENE | 8 | 0.906 | 104.1 | 100% |
| 139 | HCHO | 1 | 0.815 | 30.05 | 92% |
| 205 | MEOH | 1 | 0.7914 | 32.04 | 100% |

0.8 ppm. The exact calculated concentrations were determined by flow measurements with soap-bubble meters for the air and NO. The measured concentrations were plotted against the calculated concentration. All data were fit to a straight line with the least-squares method. The data is plotted in Figure 1 and is shown in Table 6. Agreement between the sources is excellent. The values assigned to these tanks determine the absolute accuracy of our reported $NO_x$ and $O_3$ data.

### Hydrocarbon Sources

Because there is much less of a distinction between primary and working sources for hydrocarbons than for $NO_x$ and $O_3$ sources, the comparison of primary hydrocarbon sources will be discussed below in the next section on transfer standards.

## Transfer Calibration to working "AUTOCAL" Sources

### NOx and O3 Calibration Sources

Experience and analysis of past calibration data indicates that calibration factors estimated from the results of the "manually" performed gas-phase titration method vary more than the calibration factors obtained from the automatic span checks using low concentration sources. But when the manual values are averaged, they yield the same results. The low concentration sources are convenient, but require careful characterization, since their concentration decreases slightly during the run season. Our experience and analysis also shows that the instruments are more stable if the zero and span settings are not adjusted. Therefore, the following strategy is followed to maximize the quality of the data from these instruments.

The $NO_x$ and $O_3$ instruments are not adjusted after the initial start-up at the beginning of the experimental season. Manual gas-phase titration calibrations are performed to estimate calibration factors for the instruments throughout the experimental season. The low concentration sources are used twice a day. The responses are plotted for the entire run season to establish a decay rate for the low concentration sources. The manual calibration factors establish the concentrations of these low concentration sources at the beginning of the season. The calibrated responses from the low concentration sources are then used to calibrate the instruments. The flowchart illustrating the procedures associated with the transfer of $NO_x$ and $O_3$ calibrations is shown in Figure 2.

### Manual Gas Phase Titration

The manual Gas Phase Titration calibrations are performed occasionally throughout the season as discussed above. The technique is the EPA reference method as

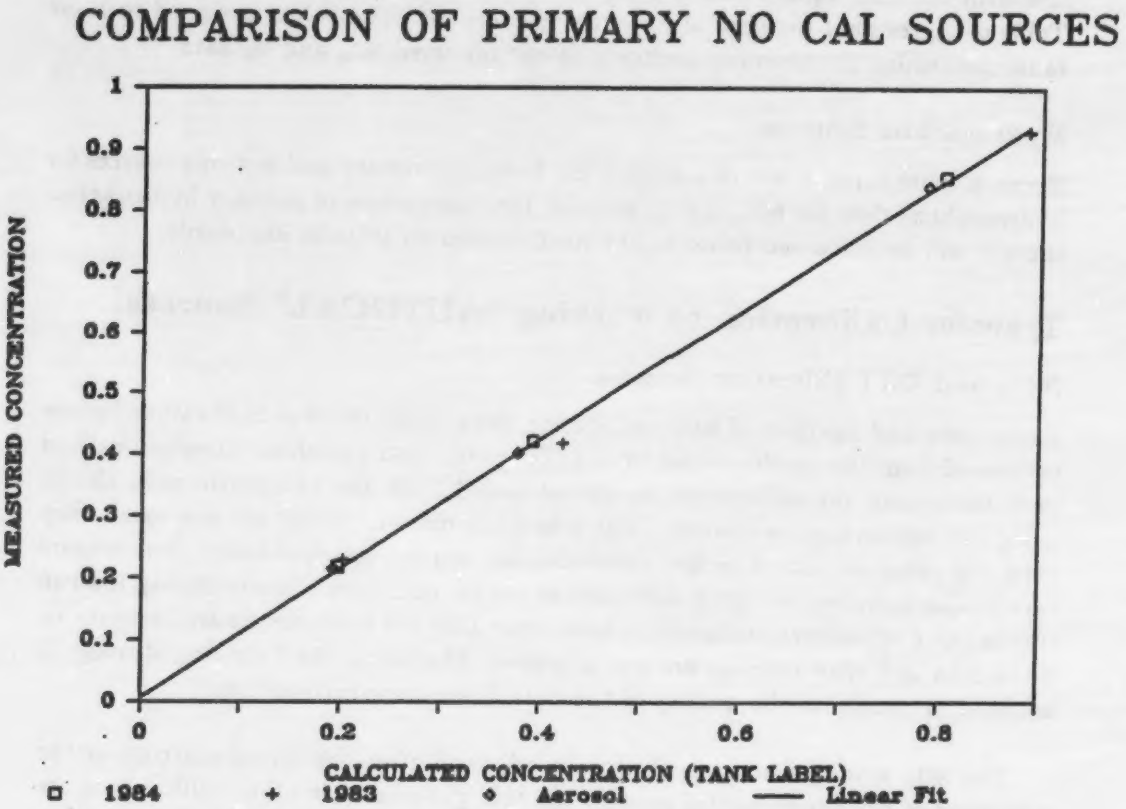


**Figure 1. Comparison of Primary NO Calibration Sources**

## Table 6. Comparison of Primary NO Calibration Sources

| TANK | CALC. CONC. | ESTIMATE CONC. | MEASURED CONC. | DELTA CONC. | PERCENT |
|---|---|---|---|---|---|
| 1 | 0.197 | 0.213 | 0.218 | 0.005 | 2.3% |
| 1984 | 0.392 | 0.418 | 0.423 | 0.005 | 1.2% |
| 52.4 ppm | 0.803 | 0.849 | 0.855 | 0.006 | 0.7% |
| 2 | 0.202 | 0.218 | 0.229 | 0.011 | 4.8% |
| 1983 | 0.422 | 0.449 | 0.419 | -0.030 | 6.7% |
| 46 ppm | 0.886 | 0.936 | 0.930 | -0.006 | 0.7% |
| 3 | 0.192 | 0.208 | 0.215 | 0.007 | 3.4% |
| Aerosol Project | 0.377 | 0.402 | 0.403 | 0.001 | 0.2% |
| 52.6 ppm | 0.786 | 0.831 | 0.840 | 0.009 | 1.0% |
|  |  |  |  | ave | 2.3% |

described in the CFR[3].

This calibration technique is based upon the rapid gas phase reaction between NO and $O_3$ to produce stoichiometric quantities of $NO_2$. The quantitative nature of this reaction is such that when the NO concentration is known (primary calibration standard), the concentration of $NO_2$ and $O_3$ can be determined. $O_3$ is added to excess NO in a dynamic calibration system, and the $NO/NO_X/NO_2$ analyzer is used as an indicator of changes in NO concentration. Upon the addition of $O_3$, the decrease in NO concentration observed on the calibrated NO channel is equivalent to the concentration of $NO_2$ produced and $O_3$ consumed.

### *Calibration Factors from Primary Sources*

Each "manual" calibration is processed with the aid of an electronic form implemented with LOTUS 123 on an IBM PC called MANCALSH.WKS in Figure 2 (see figure Figure 3. Information is transfered from the paper form filled in during the gas phase titration calibration procedure. The results of each manual calibration are inspected for notes of problems that were encountered, such as odd or unstable readings. The electronic form assures that the calculations are performed correctly. The completed form is printed out and the file is saved on diskette and backed up to another diskette, thus resulting in at least four sources of the calibration data.

Another LOTUS 123 electronic form and database is used to collect the final calibration factors for all calibrations (called MANCAL.WKS in Figure 2). Output from this worksheet is shown in Figure 4. The data are fitted with a straight line using a least-squares method. The data and the straight line fit are plotted as a function of date; these are shown in Figure 5. The plots are used to visually inspect the data for trends and large variations. If necessary, the individual calculation electronic forms can be inspected for errors in transfering data. The original paper form can also be examined. If there are problems, the data in the database may be invalidated.

If no trend is observed, the calibration factors are simply averaged for the season to estimate the true calibration factor for the instrument. Analysis of manual calibrations performed over many years by many people show variation by human error but usually no trend. If a trend were observed, the calibration factor for a particular time of interest would be estimated by a least-squares estimate through the calibration data points.

### *Calibration of AUTOCAL Sources - Transfer Standards*

The response and zero data from the AUTOCAL procedures (NO, $NO_X$, and $O_3$) are plotted and listed using a DATATRIEVE database. The first QA step is to investigate the large variations or odd values. Sometimes a calibration was not conducted and regular experimental data was processed as a calibration. A regression is calculated to estimate the decay rate and to estimate the intercept (correct response) at the beginning of the season or start of a new span check tank. The average (or if a trend was observed, the appropriate time specific) manual calibration factor is used to calculate the true concentrations of the AUTOCAL calibration sources from the responses at these times (see bottom of Figure 4and discussion of routine $NO_x$ and $O_3$ calibrations for final report of AUTOCAL calibration factors).

### Hydrocarbon Sources

A procedure similar to that performed for the different NO and $O_3$ calibration sources was performed for the hydrocarbon calibration sources. The comparison was far more complex because of the large number of species and different sources utilized. Five commercially prepared tanks purchased by UNC were compared and analyzed. Two additional well-characterized (several years history) tanks which are part of an on-going study of commercial HC calibration sources were borrowed from RTI. A low concentration tank was prepared from one of the purchased tanks. These were also compared. Liquid injections into the smog chamber used as calibration sources were also compared with these tank sources. The low concentration tank was calibrated as a working AUTOCAL source. All of the tanks, however, were used occassionally for calibration. A list of the sources that were compared is given in Table 7.

The borrowed RTI tanks were considered to be an absolute standard. The values of the other calibration sources were "analyzed" based on the RTI tanks as the primary standard. In most cases the final analyzed values for all compounds for all sources were within a few percent of the manufacturers reported concentrations and the liquid injected sources from the UNC chamber. Only one compound (2-methyl-1,3-butadiene ) was outside of the manufacturers stated uncertainty. This compound is not important to the present research program.

The intercomparisons of the HC sources was performed with a LOTUS 123 spreadsheet on an IBM PC. The spreadsheet is listed in Appendix B.

Table 8 shows the agreement with the manufacturers analysis after "validating" the tanks with the RTI NBS-traceable tanks (see Table 7). For each tank, the average and standard deviation of the ratio of the "validated" to manufacturers stated concentration for each species in the tank are listed. The range of agreement is 0.94 to 0.99 with a mean of 0.963 and a relative standard deviation of 1.8 percent; the

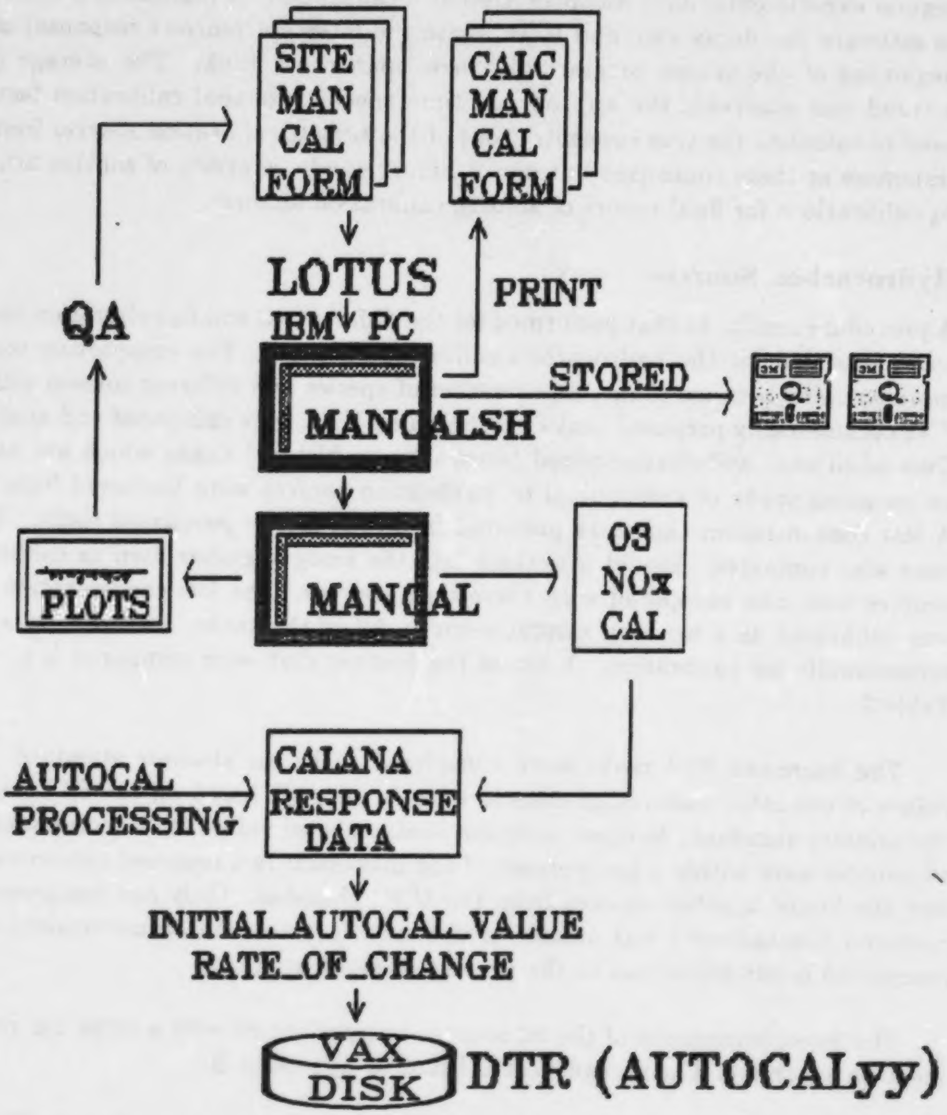

SITE MAN CAL FORM
CALC MAN CAL FORM
LOTUS
IBM PC
PRINT
QA
STORED
MANCALSH
PLOTS
MANCAL
O3 NOx CAL
AUTOCAL PROCESSING
CALANA RESPONSE DATA
INITIAL_AUTOCAL_VALUE
RATE_OF_CHANGE
VAX DISK
DTR (AUTOCALyy)

**Figure 2.** $NO_x$ and $O_3$ Cal Processing Flowchart

```
 NO-O3 Calibration Data Sheet        DATE 8/6/85     NAME Suedbeck
                                          --------        -------------------------
 Air Flow:
  volume  0.485    time   0.221   0.223   0.222   0.223   0.221     av: 0.22200
         --------        ------- ------- ------- ------- -------        --------
                                                         air flow =     2.18468
                                                                         --------
 NO Cal Tank Flow(tank and O3 turned on __30_ min before flow rate measurements)
  volume    0.01    time   0.361   0.361   0.359   0.360   0.361     av: 0.36040
         --------        ------- ------- ------- ------- -------        --------
                                                       NO flow =        0.02775
                                                                         --------
                                            _                    _
                                            !       NO Flow        !
 Predicted NO:    tnk conc 52.453           !       0.02775        !          0.65783
                           -------     x    ! ------------------- !     =    --------
                                            !       2.21243        !
                                            !_    NO + Air Flow   _!

                                                    0.01254
                                                    --------
          ZERO READING !ZERO POT SETTING               SPAN READING !SPAN POT SETTING
         ______________!________________              ______________!________________
         before/ after! !before/ after!               before/ after! !before/ after!
   NO (1)  -0.015       !    214                 (2)   0.586         !   604
         ------- -------!------- -------              ------- -------!------- -------
  NO2 (1)  -0.009       !    35                  (2)  -0.002         !   572
         ------- -------!------- -------              ------- -------!------- -------
  NOX (1)  -0.018       !    181                 (2)   0.642         !   714
         ------- -------!------- -------              ------- -------!------- -------
   O3 (2)   0.001       !     0                                      !   230
         ------- -------!------- -------                             !------- -------
         ! enter NA if no adjustment made to pot settings
         (1) zero air with H2O (purafil)           (2) with NO added

 O3 SLIDE OUT AND TITRATION BEGINS!

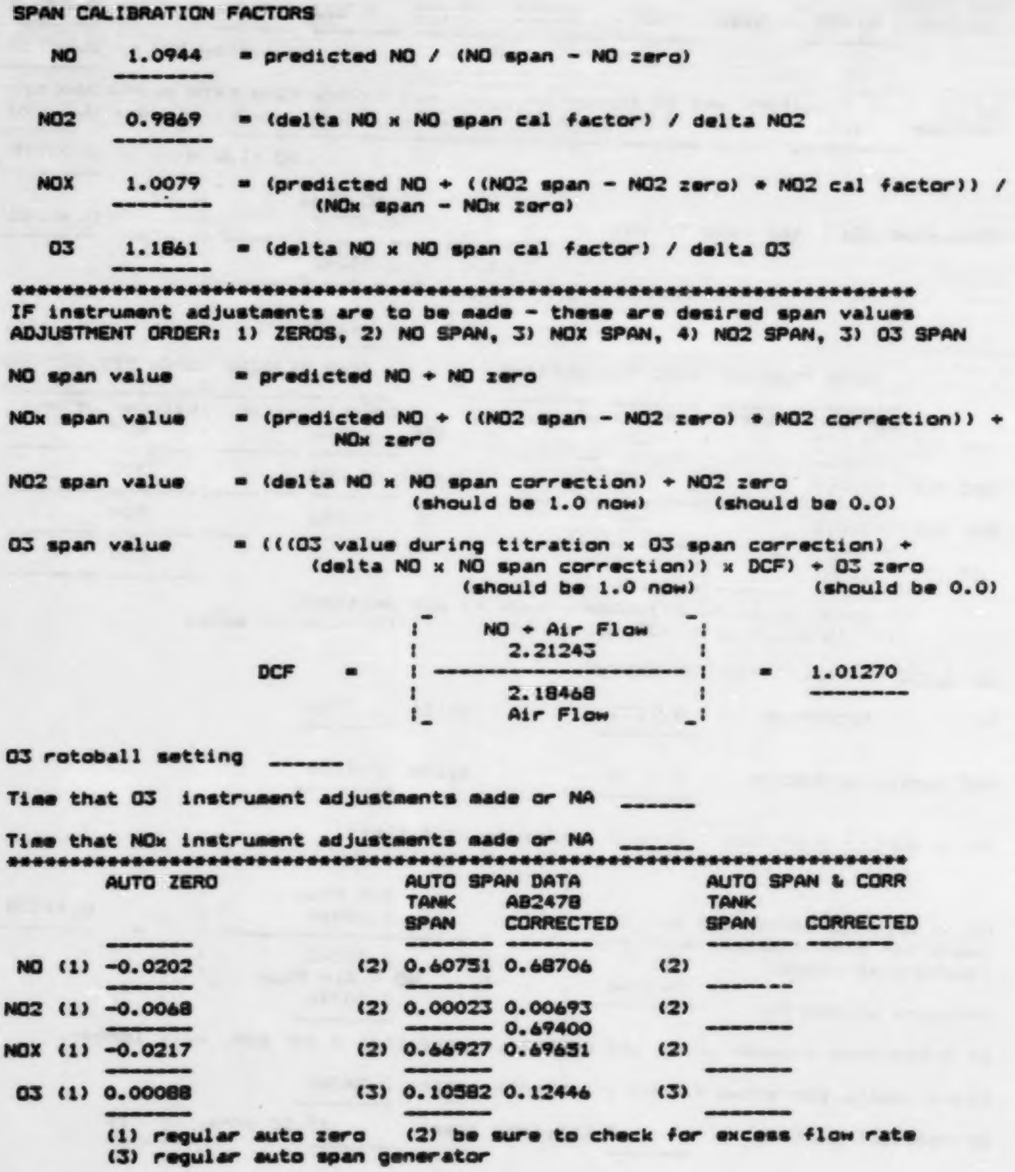
 NO during titration       0.2133            delta  0.3724
                           --------                 --------

 NO2 during titration      0.4112            delta  0.4130
                           --------                 --------

 Ozone during titration    0.0665  (measure at outlet)
                           --------
                                           _                   _
                                           !      Air Flow      !
 Ozone with NO TURNED OFF 0.4153           !      2.18468       !          0.41009
 (wait for stable value) --------     x    ! ------------------ !     =    --------
 (measure at inlet)                        !      2.21243       !
                          0.4162           !_   NO + Air Flow  _!
 (measure at outlet)     --------                 0.98746
                                                  --------
 If difference between inlet and outlet is more than a few ppb, wait longer.

 Ozone (delta corrected for NO dilution):  delta 0.34363
                                                 --------
 O3 rotoball setting            3 Ethylene pres.      15 O2 pres.      20
                          -------              -------            -------
```

Figure 3. LOTUS Spreadsheet for Manual Cal Processing



```
SPAN CALIBRATION FACTORS

   NO    1.0944   = predicted NO / (NO span - NO zero)
         --------
  NO2    0.9869   = (delta NO x NO span cal factor) / delta NO2
         --------
  NOX    1.0079   = (predicted NO + ((NO2 span - NO2 zero) * NO2 cal factor)) /
         --------         (NOx span - NOx zero)

   O3    1.1861   = (delta NO x NO span cal factor) / delta O3
         --------
**********************************************************************
IF instrument adjustments are to be made - these are desired span values
ADJUSTMENT ORDER: 1) ZEROS, 2) NO SPAN, 3) NOX SPAN, 4) NO2 SPAN, 3) O3 SPAN

NO span value      = predicted NO + NO zero

NOx span value     = (predicted NO + ((NO2 span - NO2 zero) * NO2 correction)) +
                          NOx zero

NO2 span value     = (delta NO x NO span correction) + NO2 zero
                             (should be 1.0 now)      (should be 0.0)

O3 span value      = (((O3 value during titration x O3 span correction) +
                         (delta NO x NO span correction)) x DCF) + O3 zero
                                (should be 1.0 now)          (should be 0.0)
                                 _                     _
                                !    NO + Air Flow      !
                                !       2.21243         !
                    DCF    =    ! -------------------- !    =    1.01270
                                !       2.18468         !         --------
                                !_      Air Flow       _!

O3 rotoball setting  ______

Time that O3  instrument adjustments made or NA  ______

Time that NOx instrument adjustments made or NA  ______
**********************************************************************
          AUTO ZERO                    AUTO SPAN DATA            AUTO SPAN & CORR
                                       TANK    AB2478            TANK
                                       SPAN    CORRECTED         SPAN    CORRECTED
          -------                      ------- -------           ------- -------
  NO (1) -0.0202                   (2) 0.60751 0.68706       (2)
          -------                      -------                   -------
 NO2 (1) -0.0068                   (2) 0.00023 0.00693       (2)
          -------                      ------- 0.69400           -------
 NOX (1) -0.0217                   (2) 0.66927 0.69651       (2)
          -------                      -------                   -------
  O3 (1) 0.00088                   (3) 0.10582 0.12446       (3)
          -------                      -------                   -------
          (1) regular auto zero    (2) be sure to check for excess flow rate
          (3) regular auto span generator
```

Figure 3, cont. LOTUS Spreadsheet for Manual Cal Processing.

MANUAL CALIBRATIONS

21-May-85 - last update

52.4528 ppm NO Tank

| | | NO | | | NOx | | | O3 | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Cal Date | day zero 02-Jul-84 | real | delta response | real/ response | real | delta response | real/ response | real | delta response | real/ response |
| 02-Jul-84 | 0 | 0.7482 | 0.7710 | 0.9704 | 0.7521 | 0.8170 | 0.9205 | 0.2640 | 0.2344 | 1.1260 |
| 10-Jul-84 | 8 | 0.7698 | 0.8360 | 0.9208 | 0.7707 | 0.8810 | 0.8747 | 0.2385 | 0.2403 | 0.9926 |
| 16-Jul-84 | 14 | 0.78355 | 0.8540 | 0.9175 | 0.7836 | 0.9000 | 0.8706 | 0.2340 | 0.2520 | 0.9284 |
| 18-Jul-84 | 16 | | | 0.9515 | | | | | | |
| 18-Jul-84 | 16 | | | 0.9615 | | | | | | |
| 18-Jul-84 | 16 | | | 0.9443 | | | | | | |
| 29-Aug-84 | 58 | 0.7835 | 0.8430 | 0.9294 | 0.7835 | 0.8840 | 0.8863 | 0.2172 | 0.2387 | 0.9100 |

LEAST SQUARES FOR SPAN NO

| N | X | Y | N*X | N*Y | YDEV2 | est y | X2 | Y2 | XY | rel std dev |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0.97042801 | 0 | 0.97042801 | 0.00079638 | 0.9491 | 0 | 0.94173053 | 0 | 1.13 |
| 1 | 8 | 0.92080143 | 8 | 0.92080143 | 0.00045822 | 0.9461 | 64 | 0.84787528 | 7.36641148 | -1.34 |
| 1 | 14 | 0.91750585 | 14 | 0.91750585 | 0.00061018 | 0.9438 | 196 | 0.84181699 | 12.8450819 | -1.39 |
| 1 | 16 | 0.9515 | 16 | 0.9515 | 0.00008634 | 0.9431 | 256 | 0.90535225 | 15.224 | 0.45 |
| 1 | 16 | 0.9615 | 16 | 0.9615 | 0.00037219 | 0.9431 | 256 | 0.92448225 | 15.384 | 0.98 |
| 1 | 16 | 0.9443 | 16 | 0.9443 | 0.00000437 | 0.9431 | 256 | 0.89170249 | 15.1088 | 0.07 |
| 1 | 58 | 0.92941874 | 58 | 0.92941874 | 0.00016355 | 0.9273 | 3364 | 0.86381919 | 53.9062870 | 0.11 |
| 7 | | | 128 | 6.59545404 | 0.00249127 | | 4392 | 6.21677899 | 119.834580 | |

AVE CAL: 0.94220772
XBAR: 18.2857142
SD: 0.01886519
SLOPE: -3.744E-04
INTER: 0.94905347
R2: 0.11541280

LEAST SQUARES FOR SPAN NOx

| N | X | Y | N*X | N*Y | YDEV2 | est y | X2 | Y2 | XY | rel std dev |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0.92050183 | 0 | 0.92050183 | 0.00047114 | 0.8925 | 0 | 0.84732363 | 0 | 0.49 |
| 1 | 8 | 0.87474460 | 8 | 0.87474460 | 0.00455127 | 0.8907 | 64 | 0.76517812 | 6.99795686 | -0.28 |
| 1 | 14 | 0.87061111 | 14 | 0.87061111 | 0.00512607 | 0.8894 | 196 | 0.75796370 | 12.1885555 | -0.33 |
| 1 | 58 | 0.88631221 | 58 | 0.88631221 | 0.00312430 | 0.8796 | 3364 | 0.78554934 | 51.4061085 | 0.12 |
| 4 | | | 80 | 3.55216977 | 0.01327279 | | 3624 | 3.15601481 | 70.5926210 | |

AVE CAL: 0.88804244
XBAR: 20
SD: 0.05760381
SLOPE: -2.227E-04
INTER: 0.89249673
R2: 0.06530589

**Figure 4.** LOTUS Analysis Spreadsheet of Manual Cal

```
LEAST SQUARES FOR SPAN O3
       N          X          Y         N*X         N*Y       YDEV2    est y           X2          Y2           XY rel std dev
----------------------------------------------------------------------------------------------------------------------------
       1          0 1.12601851           0 1.12601851 0.03378640     1.0428            0 1.26791769           0       0.86
       1         -8 0.99263298           8 0.99263298 0.00254270     1.0214           64 0.98532023 7.94106384      -0.30
       1         14 0.92837585          14 0.92837585 0.00019132     1.0053          196 0.86188173 12.9972620      -0.79
       1         58 0.91000502          58 0.91000502 0.00103701     0.8875         3364 0.82810915 52.7802916       0.23
----------------------------------------------------------------------------------------------------------------------------
       4                                80 3.95703238 0.03755744                  3624 3.94322881 73.7186174

                              AVE CAL:   0.98925809                  SD:         0.09689872 SLOPE:      -2.679E-03
                              XBAR:         20.0000                                         INTER:      1.04283546
                                                                                            R2:         0.50605026


AVE CAL:    Auto Tank 1 : 6/21 to 9/1                                  Auto Tank 2 : 9/1 to 10/16

--------  ---------------------------                                ---------------------------
   NO     response1 CAL VALUE              decay*                    response2 CAL VALUE                decay*
 0.94221   0.30515   0.28751               -4.485E-05                  0.70602   0.66522              -5.607E-04

                                     0.53% agreement                                                -0.42% agreement
   NOx    response1 CAL VALUE              decay*                    response2 CAL VALUE                decay*
 0.88804   0.32207   0.28601               -5.304E-05                  0.75224   0.66802              -3.688E-04

            Auto Cal Gen : 5/30 to 11/6

          ---------------------------
   O3      response CAL VALUE              decay*
 0.98926   0.12218   0.12087               -7.179E-05


response1 -response value for 21-JUN-84 determined from least squares regression of response data

response2 -response value for 1-SEP-84 determined from least squares regression of response data

decay*    -from least squares regression of response data

CAL VALUE -VALUE ENTERED INTO AUTOCAL DATABASE TO GENERATE DAILY CAL FACTORS
```

**Figure 4, cont.** LOTUS Analysis Spreadsheet Manual Cal Plots.

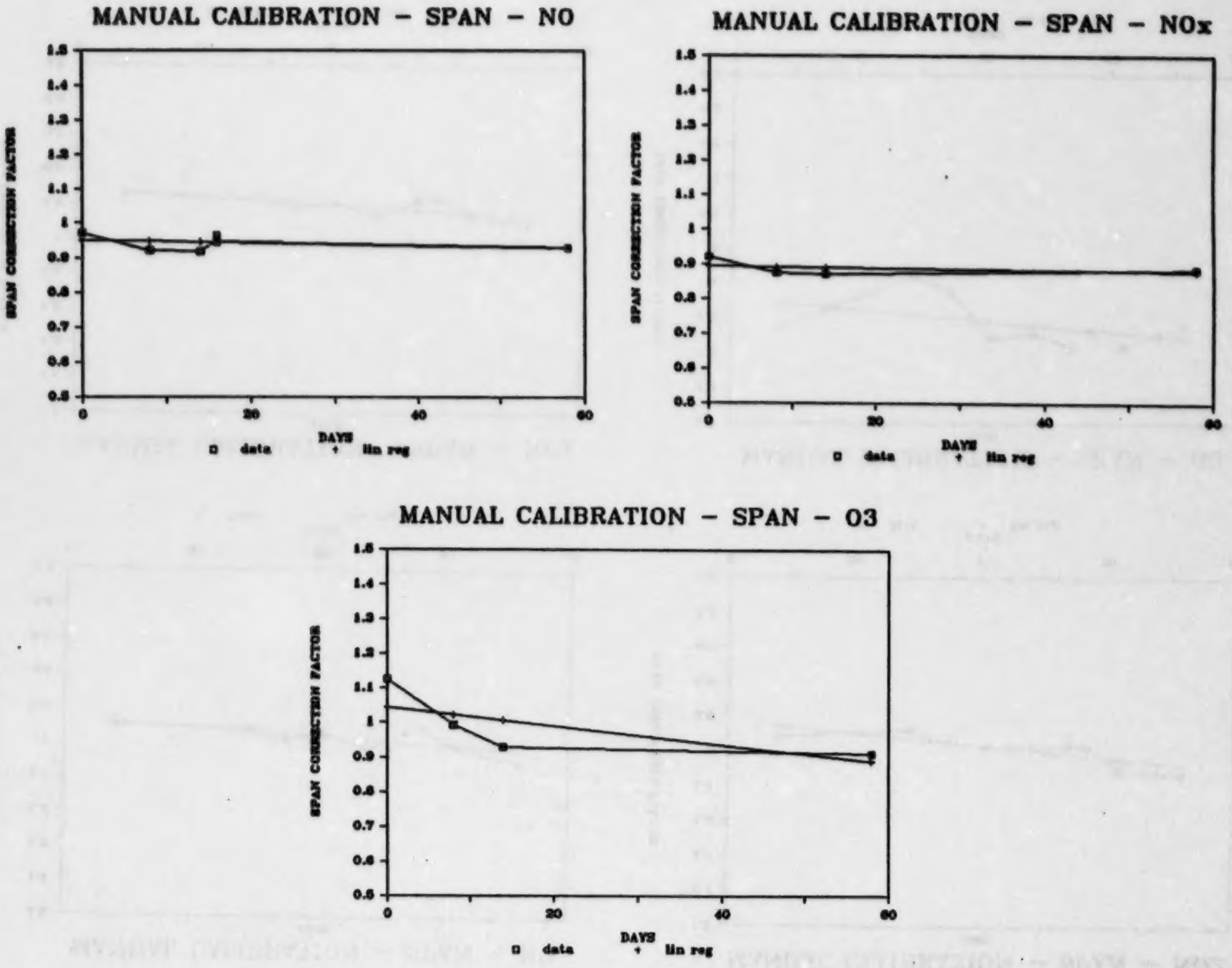


Figure 5. LOTUS Analysis Spreadsheet of Manual Cal Plots

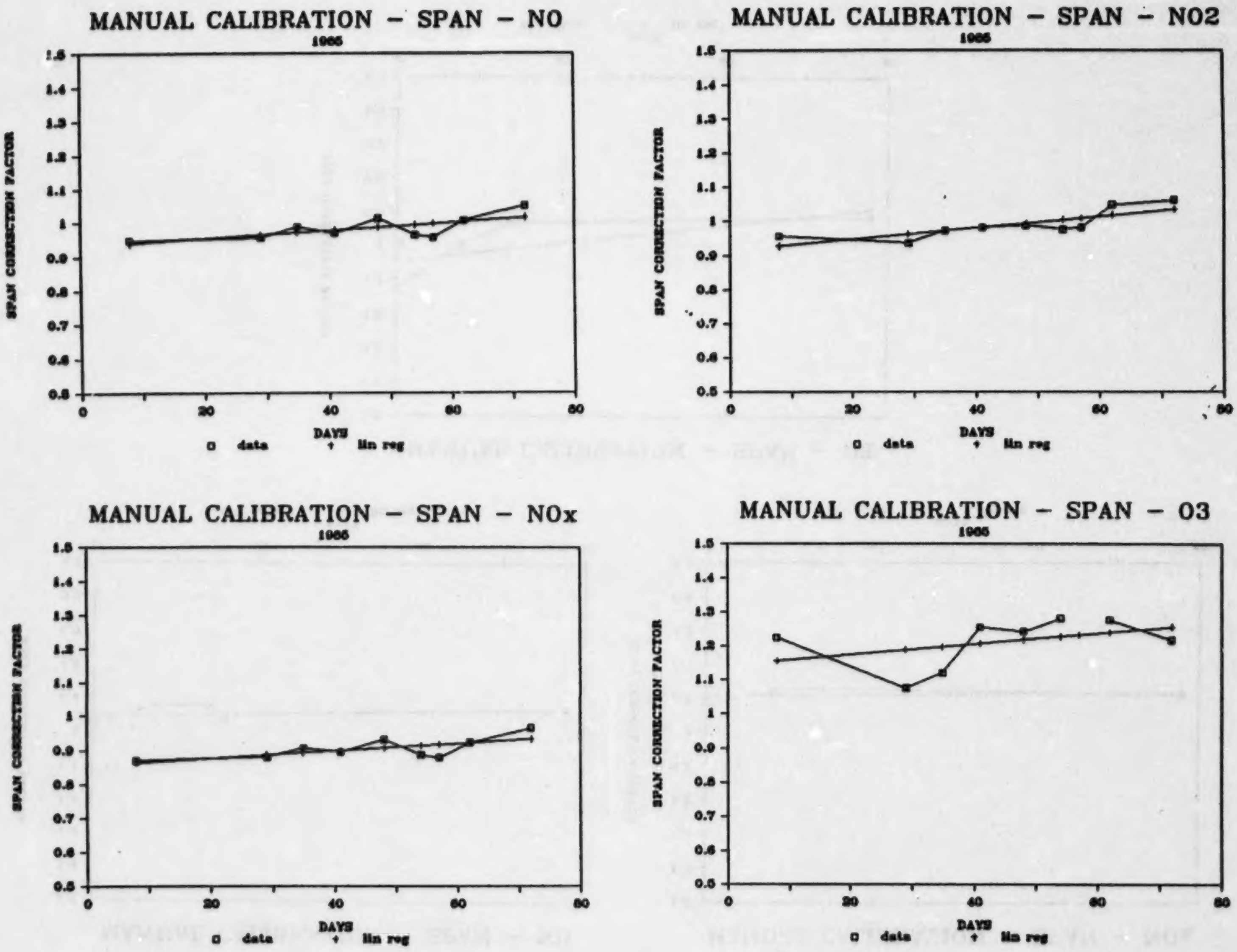


Figure 5, cont. LOTUS Analysis Spreadsheet of Manual Cal.

largest individual relative deviation from the average is 2.5 percent. The agreement between the standard tanks and the RTI tanks is very good. The absolute accuracy of the hydrocarbon calibrations depends directly upon the concentrations assigned to these tanks.

### Table 7. Intercomparisons Among Sources

| Source | Source | Date |
|---|---|---|
| RTI ethylene | AIRCO | 8/1-2 |
| RTI propylene | AIRCO | 8/1-2 |
| | | |
| AIRCO | LOWMW (Hi Conc) | 7/18 |
| AIRCO | HIMW (Hi Conc) | 7/18 |
| | | |
| AIRCO | LIQ STD 8/14 | 8/14 |
| AIRCO | HIMW (Hi Conc) | 8/14 |
| LIQ STD 8/14 (C/area) | HIMW (Hi Conc) | 8/14 |
| LIQ STD 8/14 (C/inch) | HIMW (Hi Conc) | 8/14 |
| | | |
| LOWMW (Hi Conc) | LOWMW (Lo Conc) | 7/13 |
| | | |
| LOWMW (Hi Conc) | HIMW (Hi Conc) | 5/30 |
| LOWMW (Hi Conc) | 82HCCALMIX | 5/30 |
| | | |
| LOWMW (Hi Conc) | SCOTTTANK | 10/5 |
| HIMW (Hi Conc) | SCOTTTANK | 10/5 |
| LOWMW (Lo Conc) | SCOTTTANK | 10/5 |
| | | |
| LOWMW (Lo Conc) | SCOTTTANK | 8/17 |
| AIRCO | SCOTTTANK | 8/17 |

### Table 8. Comparison of Primary HC Calibration Sources

| OCS ID | SOURCE | ANALYZED/ MANUFACTURER avg | std | DEV | REL DEV | ABS REL DEV |
|---|---|---|---|---|---|---|
| 1 | 82HC | 0.971 | 0.126 | 0.008 | 0.8% | 0.8% |
| 108 | HMWHC | 0.985 | 0.047 | 0.022 | 2.3% | 2.3% |
| 109 | LMWHC | 0.956 | 0.034 | -0.007 | -0.7% | 0.7% |
| 112 | AIRCO | 0.939 | 0.101 | -0.024 | -2.5% | 2.5% |
| | ave | 0.963 | 0.077 | | | 1.6% |
| | std | 0.017 | 0.038 | | | 0.8% |
| | rel std | 1.8% | | | | |

## Routine NOx and O3 Calibrations Methods

This section describes the types of calibration methods routinely performed. The section "Calibration Data Processing" describes how the data are processed, including the QA steps. The calibration reports are included or refer to appendices of calibration reports.

### Automatic Source Sampling

The transfer technique to characterize the AUTOCAL sources for $NO_x$ and $O_3$ was described above. Before and after every experiment, these sources plus the AUTOZEROs are used to calibrate the instruments by scheduling 30 minutes to sample from the span sources and from the zero sources by computer control (0200-0230 EDT, 1800-1830 EDT for AUTOZERO; 0230-0300 EDT, 1830-1900 EDT for AUTOSPAN). The two low concentration NO tanks used for AUTOCAL sources are listed in Table 2. The generator built into the $O_3$ monitor is used for the $O_3$ AUTOCAL source.

DATATRIEVE is used to maintain an AUTOCAL database. In this database, the decay rates and the initial concentrations at the beginning of the season are used to estimate the concentration of the span sources for each AUTOCAL performed. A database procedure PRINT_CALS_AND_FACTORS computes calibration factors from the AUTOCAL response and the computed tank concentration.

## Routine HC Calibrations

### Automatic Source Sampling

Routine HC calibrations were performed automatically before every experiment. The GCs are activated several hours before injections and are allowed to produce several chromatograms. A timer switches on the calibration source tank connected to a calibration manifold at approximately 0300 EDT. The flowrate is adjusted to provide an excess which is vented. The timer also switches a three-way valve to change the GCs from the chamber sample manifold to the calibration source manifold. The "low concentration" tank listed in Table 3 and discussed above was the source most commonly used for an AUTOCAL, however other tanks listed in the table were sometimes used. This would normally be when the presence of a morning site operator was required many hours before sunrise. Sometimes calibrations were performed after an experiment when a wider range of calibration species were desired. The site operator indicated on the instrument checklist that a calibration was performed. When the run is logged in later in the data processing office, these notes of calibrations performed will be logged into the calibration database (discussed below).

### Manual Precision Liquid Injections

More extensive calibrations were performed on days that were poor for performing an experiment (poor sun or rain forecast). On these "CAL" days, several tanks would be used for calibrating. More importantly, liquid standards could be injected into the unused chamber for calibrating compounds with vapor pressures too great to be stored in pressurized cylinders (*e.g.*1, 2,4-trimethylbenzene). These calibration data are stored in a "CAL" folder. The presence of the "CAL" folder and a calendar entry indicating a "CAL DAY" will trigger the processing of a calibration that was not performed during an experiment.

Liquid injections of reasonably large amounts (100's of $\mu$l) used to produce initial injections for a smog chamber experiment were usually processed as calibration sources also. The project coordinator decides if the injections are appropriate as a calibration source and then logs in the calibration.

#### *Injection Calibration Procedures*

The chamber is usually vented more than 10 hours before injections are made. Hamilton "Standard Microliter " gas chromatography syringes are used to inject known volumes (in 10's to 100's $\mu$l) range) into the smog chamber. Stated accuracy is 1% of the syringe volume. The temperature is recorded for concentration calculations. All data are recorded on the stripchart or by a special note on the RUN SHEET or INSTRUMENT CHECKLIST.

Injection calibration data are transfered to the Official Calibration Source form (OCS), then to the electronic OCSIC84 form which performs ideal gas law calculations, using the amount injected and the chamber volume. The electronic form automatically looks up density, carbon number, MW *etc.*All calculations are thus recorded. Errors (from improper data transfer or calculation) are therefore minimized.

The determination of chamber volume was by a "strapping" technique. The dimensions of the chamber were carefully measured and used to calculate the volume. Several people have independently made these measurements with less than 1.5% variation in volume.

## Meteorological Sensor Calibrations

### Solar/UV radiation Calibrations

Two sets of both the Eppley Black and White Pyranometer (Total Solar Radiation) and Eppley Ultra-Violet Radiometer (Ultraviolet) sensors are used. One set is used continuously and the other set is reserved as the References. Both sets are calibrated by Eppley. The continuous sensors are sent back to Eppley annually for recalibration. At Epply, the total solar radiation sensor is compared with the Eppley group of reference standards at approximately one half a solar constant. The UV sensor is calibrated by comparison with an Eppley standard of spectral irradiance lamp.

### Temperature Calibrations

The temperature thermistors are checked against an ice bath and a water bath near normal high afternoon temperature, measured with a general laboratory mercury thermometer.

### Dewpoint Calibrations

There is no direct calibration technique for the dewpoint monitor. The sensor is a high precision point thermometer sensor. The electronics of the instrument must be frequently adjusted to balance the sensor bridge. The detector must also be cleaned routinely. The dewpoint meter is checked by monitoring the saturated air pulled through a water bubbler of known temperature. Response to dry air (air pulled through Drierite) tests for proper cooling circuit operation needed to reach low dewpoints.

## Flowrate Measurements - Calibration

Accurate flowrates are required for the manual gas phase titration method for calibrating $NO_x$ and $O_3$ and for making injections into the smog chamber. The primary standards and routine flowrate measuring devices are a series of 10, 100, 1000, and 2000 milliliter soap bubble flowmeters. The volume of the soap bubble tubes was determined by measuring water volume in NBS calibrated graduated cylinders. A four place digital stopwatch is used for timing.

## Time Measurement - Clock Calibration

All times reported are Eastern Daylight Time, even during winter. The main system clock is housed within the computer. Time is set at the beginning of the run season against standard time reported at the local weather bureau at the Regional Airport. This time is verified several times during the year. Stripcharts are marked at the beginning and throughout the experiment with time read from the computer clock.

## Calibration Documentation and Processing Databases

A formal system has been developed to document and track the processing of the large calibration database. This is important to a QA program to assure that all data is processed and utilized. Various paper and electronic forms, calendars, notebooks, and computer databases are utilized. Forms help assure consistency and completeness. Electronic forms allow for ease of organization, manipulation, retrieval, and analysis. Some of the form fields are actually computed internal to the form.

### Paper Forms

*Run and Calibration Calendars*

Calendars at both the site and the office in the School of Public Health are used to record days on which experiments were conducted. These entries also indicate days on which only calibrations were performed.

*Run Folder Inventory Check Lists*

Instrument Checklists are filled out for each experiment. These lists identify the calibrations that were performed (see Appendix A).

### *Stripcharts*

Stripcharts from an experiment identify the calibrations that were performed, the calibration source, the chart attenuation, the chamber temperature, and the number of microliters that were injected.

### *Manual $NO_x/O_3$ Calibration Form*

Paper forms are used to record manually performed calibrations. These are filled out at the site and transported to the data processing office where they are transfered to electronic form (see below) and stored.

### *Official Calibration Source Form*

All information, including the calibration source concentration used for a calibration, is recorded on Official Calibration Source (OCS) forms (see Figure 6). Information concerned with several stages of processing and several different programs, worksheets, and databases is recorded. The calibration information comes from several sources including stripcharts and attached notes. This form has an id number. identification information, amounts and temperature, and official validated concentration. This information is further stored in a computer database described below which generates a file for processing calibration factors.

### *Calibration Pick Instructions*

A paper form is used to give and record processing instructions to Data Processors for the raw calibration response data. The location of the calibration data is recorded and the corresponding calibration sources used are identified. Notes can be made about processing status and special problems and processing instructions. Processing status is recorded on this form and concurrently in CALENTRY, a computer database for tracking processing status (see below). Figure 7 shows this form.

## Electronic Forms and Other Documentation

### *COMMAND FILE*

Command files are created at the smog chamber site on the computer used to control the experiment. Commands issued to perform auto cals can be used later to document the exact time the instruments are calibrated. Other instruments not directly controlled yet auto calibrated are identified in remarks in the command file.

# Offical Calibration Source Form

**Who is filling out this form:**______________________

**Date form filled out:** ______________________

**SOURCE INFORMATION.**

**INSTRUCTIONS:**

`ID NUMBER`:The id number is the next sequential calibration source number.

`DESCRIPTION`: examples are: `82SCOTHC`, or `STDMIX2INJ`. Please print.

`SOURCE DATE`: the date tank was acquired or the date of injection.

`SERIAL NUMBER`: the tank serial number or the initials of the injector. Please print.

**VALIDATION OF SOURCE:**

`VALIDATION DATE` The date that the source was approved.

`INITIALS` The person doing the approval.

ID NUMBER Three digits. __________

DESCRIPTION Ten chars. ______________________

SOURCE DATE dd-mmm-yy ______________

SERIAL NUMBER Ten chars. ______________

**Figure 6. Official Calibration Source Form**

**SOURCE VALUE :: one page per species.Page ________ of ________**

SPECIES NAME Full name ____________________

SPECIES NUMBER Three digits ____________

STATED CONC. 9.9999 ____________

ACTUAL CONC. 9.9999 ____________

CONC. UNITS *e.g.* ppmC ____________

---

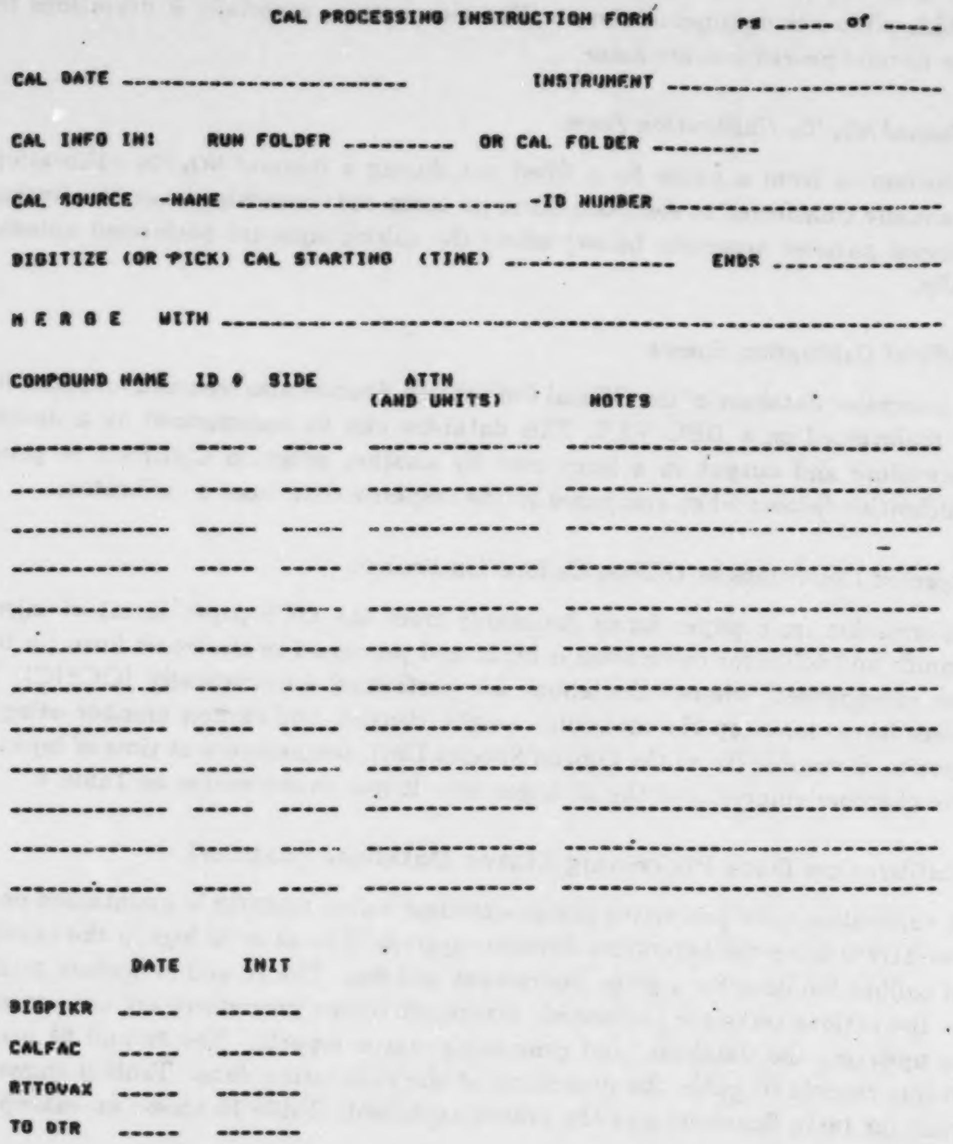
VALIDATION DATE dd-mmm-yy ____________

INITIALS ______

---

COMMENTS:

**Figure 6, cont.** **Official Calibration Source Form.**



CAL PROCESSING INSTRUCTION FORM pg ____ of ____

CAL DATE ______________________ INSTRUMENT ______________________

CAL INFO IN: RUN FOLDER _________ OR CAL FOLDER _________

CAL SOURCE -NAME ______________________ -ID NUMBER ______________________

DIGITIZE (OR PICK) CAL STARTING (TIME) ______________ ENDS ______________

MERGE WITH ______________________________________________________

| COMPOUND NAME | ID # | SIDE | ATTN (AND UNITS) | NOTES |
|---|---|---|---|---|
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |
| ____________ | _____ | _____ | _____________ | ______________________ |

| | DATE | INIT |
|---|---|---|
| DIGPIKR | _____ | _______ |
| CALFAC | _____ | _______ |
| RTTOVAX | _____ | _______ |
| TO DTR | _____ | _______ |

**Figure 7. Cal Pick Instruction Form**

### *REMARKS FILE from Computer DA system*

Another file created during the experiment by the computer is the remarks file which often has comments about calibration events, especially if deviations from the normal procedures are made.

### *Manual $NO_x/O_3$ Calibration Form*

Information from a paper form filled out during a manual $NO_x/O_3$ calibration is manually transferred to electronic form (in LOTUS 123 spreadsheet, see description of general purpose programs below) where the calculations are performed automatically.

### *Official Calibration Source*

A computer database of the Official Calibration Sources also recorded on paper form is maintained on a DEC VAX. This database can be summarized by a database procedure and output in a form used by another program CALFAC to process calibration factors when compared to the response data from a calibration.

### *Injected Conditions as Official Calibration Sources*

Information from paper forms (primarily from the OCS paper form) of injected liquids and solids for calibration is input and processed in electronic form (in LOTUS 123 spreadsheet) where calculations are performed automatically (OCSIC). The spreadsheet looks up the molecular weight, density, and carbon number using the species id number (from the Official Species List), temperature at time of injection, the chamber volume, and the ideal gas law. It was shown earlier as Table 4.

## Calibration Data Processing Status Database (CALENTRY)

A calibration data processing status database called CALENTRY is maintained on the VAX-11/780 using the DATATRIEVE database system. The AA or PC logs in the existence of calibration data for a given instrument and day. The PC and PP update CALENTRY as the various tasks are performed. DATATRIEVE report procedures are used to assist in updating the database, and generating status reports. The PC and PP use the status reports to guide the processing of the calibration data. Table 9 shows the CALENTRY tasks flowchart and the events explained. Table 10 shows an example of the CALSUM report.

## Calibration Databases

Several calibration databases are maintained. Some double as spreadsheets to per-

# Table 9

## Processing System for Instrument Auto-Calibration Data

```
tot inst    cal analysis
      \    /           \
       !CPI!           !OCS!
           \               \
            \               \
            <DPR>----------<CFR>--(Q2V)--(DTR)--(C2L)--<CLR>--!CQA!
```

```
!sss! == stages determined by Project coordinator (PC)
<sss> == stages determined by Peak Pickers (PP)
(sss) == stages determined by Computer Techs (CT)
```

| Step | CALENTRY stages | Meaning |
|---|---|---|
| PC | CPI : CAL pick Inst | Charts marked, cal status sheet in folder |
| PP | DPR : Digpik run | Cal data digitized and R-file exists |
| PC | OCS : OCS ok | Official Cal Source exists in DTR |
| PP | CFR : CALFAC run | Cal Factor computed, Q-file created |
| CT | Q2V : Qfile to vax | Q-file moved to VAX |
| CT | DTR : DTR file updated | Cal Data added to DTR data base |
| CT | C2L : Cals to LSI | DTR CAL file loaded on LSI-11 |
| PP | CLR : CALANA run | Cal Factors analyzed |
| PC | CQA : Cal QA | Cal Factor Quality Assurance |
| PC | NTB : Not to be proc | Not to be processed |
| PC | BAD : Stop processing | Something is wrong with this run |

## Table 10. CALSUM Example

```
Count of calibrations that have reached stated stages of processing
        for METH

Total calibrations

     265

******** HC Instrument data ************

CPI DPR OCS CFR Q2V DTR C2L CLR CQA C2S NTB BAD

181 181 181 181 179 179   0   0 144   0  53   9

     Sum of CPI and NTB is  234




                  CAL PROCESSING STATUS                    6-May-1985
                                                           Page 5

        CAL                                   Calibration
        DATE  Instrument                        Steps

         Carle III GC                      CAL pick Inst
                                           Digpik run
                                           CALFAC run
    13-Jul-1984
         Carle I   GC                      CAL pick Inst
                                           Digpik run
                                           CALFAC run
         Carle II  GC                      CAL pick Inst
                                           Digpik run
                                           CALFAC run
         Carle III GC                      CAL pick Inst
                                           Digpik run
                                           CALFAC run
         CEA Formaldehyde                  CAL pick Inst
                                           Digpik run
                                           CALFAC run
    14-Jul-1984
         Carle I   GC                      CAL pick Inst
                                           Digpik run
                                           CALFAC run
         Carle II  GC                      CAL pick Inst
                                           Digpik run
                                           CALFAC run
         Carle III GC                      CAL pick Inst
                                           Digpik run
                                           CALFAC run
    16-Jul-1984
         Carle I   GC                      CAL pick Inst
                                           Digpik run
                                           CALFAC run
         Carle II  GC                      CAL pick Inst
                                           Digpik run
                                           CALFAC run
         Carle III GC                      Not to be proc
```

form calculations. The databases serve several functions. Database commands and procedures can sort by instrument and species, make plots of cal-factors vs time, perform regression and correlation calculations, convert to a common attenuation or range, output reports, output files for other programs, and in general allow us to organize, retrieve and update information easily.

### *HC Tank Calibration Source Certification Database ("CAL")*

Many different calibration sources were used for hydrocarbons. Some are "cal" tanks and others are analyzed by the manufacturer with a stated uncertainty. Liquids injected into the chamber are another calibration source. All "cal" sources were intercompared to check for consistency. Data was collected in both peak height and integrator area, and organized in a LOTUS 123 spreadsheet database. Calculations of the intercomparison were then performed (see Appendix B).

### *Official Calibration Sources (OCS) Database*

The Official Calibration Sources (OCS) Database were mentioned earlier in the electronic forms section. The database utilizes DATATRIEVE on the VAX-11/780. The database appears as a collection of forms on terminal screens which makes updating easier. Procedures have been written to generate reports (see Appendix C) and a file of the calibration source data required by the program CALFAC used to calculate the calibration factors.

### *Gas Phase Titration Database ("MANCAL" LOTUS 123 )*

The resulting calculations (calibration correction factors) processed from the raw calibration zero and response data are summarized and analyzed in another database/spreadsheet using LOTUS 123. Plots of calibration data vs time with regressions and correlation are produced easily. Trends and variation are easily recognized. Reports are quickly produced.

### $NO_x$ *and* $O_3$ *Auto-calibration Database: AUTOCAL*

The $NO_x$ and $O_3$ AUTOCAL data are maintained in a separate DATATRIEVE database. Instrument calibration zeros and responses to the AUTOCAL sources are recorded. Report procedures compare the corrected responses to the known calibration source concentration and generate and list the calibration factors, sorted by date and time of day (autocals for $NO_x$ and $O_3$ are usually performed twice a day).

### Hydrocarbon Auto-Calibration Database

Another DATATRIEVE database similar to the $NO_x$ and $O_3$ AUTOCAL database is maintained for hydrocarbon calibration data. The database is more complex because of the many more instruments which are calibrated. The database is also much larger. A calibration factor is recorded for each species. Attenuation is also recorded. Interactive report procedures can retrieve and sort calibration data by instrument, species, and date, and convert calibration data to a common attenuation. This report is the primary source of final calibration data used to process data. Another procedure outputs a file which can be read by another custom program (CALANA) which statistically analyzes calibration data for a given species instrument combination and plots the calibration history for the run season.

### Calibration Factors Used Database

Another DATATRIEVE database is used to record the calibration factors actually used to process the final experimental time-concentration data. Some interpretation and choice must be made when the statistics and the various sources of calibration factors do not agree. The PC makes a judgement based on all calibration information and chooses a calibration factor. The chosen calibration factor is kept in a separate data base. The resulting calibration factor database is maintained as a final source of information for making a choice in a calibration factor. We believe that except for rare occurences, calibration factors for most instruments do not vary much. This database is consulted to see if the calibration factor chosen varies much from those used on data from days (experiments) before and after the current experiment being processed.

## Security of Calibration Databases

There are three basic approaches to data security: inventory, retention of original data in restricted areas, and maintaining several backup copies of all data in different locations. All data are under lock at night and on weekends.

### Inventory

At the site during an experiment, the calibrations that were performed are indicated on a Instrument Checklist Form. Afterwards, before anyone is allowed to work with the run folder contents, a run folder inventory is performed which documents all data and forms. This assures that no data or documentation are lost.

### *Retention of Data*

All original data in both paper and electronic files are retained. Paper format data (all stripcharts, forms) are not allowed out of the School of Public Health office.

### *Backup of Data*

Multiple copies of data are maintained in several formats, in several locations. Backup copies of raw and final data on floppies on IBM PC are kept in several locations. LOTUS 123 worksheet files are backed up in two locations. A hardcopy (printout) of worksheet formulas using a spreadsheet AUDITOR program is kept. Backup copies of raw and final data on LSI-11 computers are maintained in several locations, including: raw data and processed data sets backed up on two diskettes, processing programs (sources) backed up on two diskettes, and whole image backup of LSI hard disk. Backup copies of final data are maintained on the VAX and are further backed-up on tapes of VAX files. There are also frequent printouts of final calibration data in notebooks. The school operates a daily, weekly, and monthly backup of VAX files with off-site vault storage for ten years for all VAX data.

## Calibration Data Processing

This section describes and illustrates the actual data processing procedures. Processing techniques are discussed separately for NO$_X$/O$_3$ and HC data, because of the different data and processing requirements and the different type of calibration sources. The databases are also maintained separately. Another important distinction is the way the different types of calibration data are transported from the smog chamber to the data processing office in the School of Public Health.

### NO$_X$ and O$_3$

#### *Manual Calibration Processing for Characterization of* AUTOCAL *Sources*

The calibration sources used for the NO$_x$ and O$_3$ monitors were discussed above. Also discussed was the relationship between the manual and auto calibrations performed. The manually performed gas phase titration calibrations are used to calibrate the auto calibration sources.

#### AUTOCAL *Data Processing*

AUTOCAL data for zeros and spans is obtained twice daily. The PDP/11-40 computer at the site initiates the calibration from a COMMAND file written by a site operator (30 minutes zero; 30 minutes span). The calibration data is recorded along with the experimental results by the computer DA system (one value every minute). Therefore the calibration data is transported along with the electronic data. Figure 8 shows a flowchart of the autocalibration data processing procedures. These tasks are mostly performed by the CT.

A computer program was written (FASTDV) to strip the calibration data from the DVM data file (see Figure 8). One file is made for every AUTOCAL performed. There are usually two autocals per day. The files are named MMDDYA.DVn where n is 1st and 2nd calibration performed. These are called "A-files". The files are backed-up on floppies. Each file is edited if necessary to eliminate readings taken in transition to the calibration value. These edited files are named MMDDYE.DVn ("E files"). These are also backed-up on floppies. They are then appended together into a file called AUTCAL.NEW. This file is appended to AUTCAL.DVM which is the "OFFICIAL" file of appended "E files", which is also backed-up on floppies.

The AUTCAL.NEW file is further processed. It is averaged to a single value for both zero and span with the program called ACALAV on the LSI-11/23. A listing of the processed averaged data is made and stored in the $NO_x/O_3$ FASTPLOT notebook. This program generates a file called ACDTR.COM which contains the processed averaged calibration data with additional DATATRIEVE commands. The file is transferred to the VAX and activated as a command procedure which causes the data to be automatically entered into the DATATRIEVE AUTOCAL database. The database also contains the characterized concentration values of the AUTOCAL sources (see discussion above). A report procedure in DATATRIEVE called PRINT_CALS_AND_FACTORS reports the original calibration data by date and time and reports the calculated correction factors. Table 11 shows the final AUTOCAL calibration factors for 1984.

## HC Processing

Processing of hydrocarbon calibration data is more complicated than processing $NO_x$ and $O_3$ calibration data. Each gas chromatograph monitors dozens, potentially hundreds, of different compounds. Each species used in an experiment requires a calibration factor for each instrument. Not every species is calibrated explicitly before every experiment. Several different calibration sources are used. Resulting calibration data must be reviewed before assigning a value for final data processing. An explicit calibration source for a compound monitored in an experiment may not exist and other techniques must be used to establish an appropriate calibration factor. The different types of calibration sources and the documentation, forms, and data bases associated with this processing were described above. This section discusses in more detail the procedures of processing the calibration data.

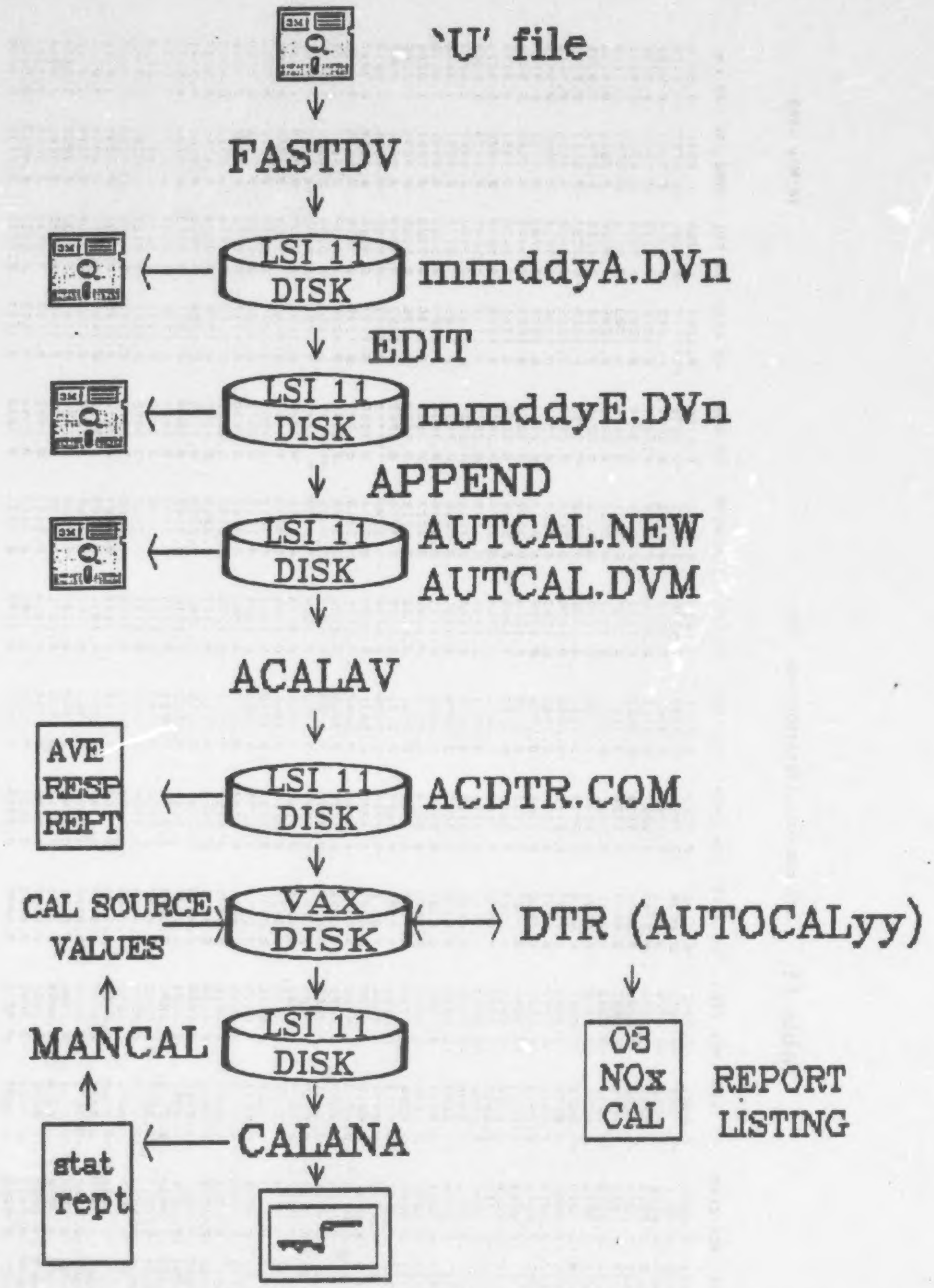

'U' file
FASTDV
LSI 11 DISK
mmddyA.DVn
EDIT
LSI 11 DISK
mmddyE.DVn
APPEND
LSI 11 DISK
AUTCAL.NEW
AUTCAL.DVM
ACALAV
AVE RESP REPT
LSI 11 DISK
ACDTR.COM
CAL SOURCE VALUES
VAX DISK
DTR (AUTOCALyy)
MANCAL
LSI 11 DISK
O3 NOx CAL
REPORT LISTING
stat rept
CALANA

Figure 8. AUTOCAL Processing Flowchart.

**Table 11.** NOX AND O3 CALIBRATIONS FOR 1984

16-May-1985

| DATE | NOX ZERO | NO ZERO | NO2 ZERO | O3 ZERO | NOX SPAN | NO SPAN | O3 SPAN | NOX RESP | NO RESP | O3 RESP | NO CAL | NOX CAL | O3 CAL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Jun23 | -0.0026 | 0.0001 | -0.0015 | -0.0140 | 0.3259 | 0.3101 | 0.1139 | 0.3285 | 0.3100 | 0.1207 | 0.9260 | 0.8746 | 0.9235 |
| Jun25 | -0.0026 | -0.0004 | -0.0010 | 0.0000 | -9.9999 | -9.9999 | -9.9999 | -9.9973 | -9.9995 | ******** | -0.0207 | -0.0207 | -0.0119 |
| Jun25 | -0.0026 | -0.0006 | -0.0004 | 0.0011 | 0.3200 | 0.3061 | 0.1253 | 0.3226 | 0.3067 | 0.1242 | 0.9364 | 0.8903 | 0.9560 |
| Jun26 | 0.0012 | 0.0025 | -0.0004 | 0.0000 | 0.3267 | 0.3116 | 0.1234 | 0.3255 | 0.3091 | 0.1276 | 0.9290 | 0.8822 | 0.9290 |
| Jun26 | -0.0014 | -0.0000 | 0.0004 | 0.0022 | 0.3190 | 0.3062 | 0.1273 | 0.3204 | 0.3070 | 0.1251 | 0.9354 | 0.8962 | 0.9404 |
| Jun27 | -0.0013 | 0.0005 | -0.0006 | 0.0007 | 0.3256 | 0.3121 | 0.1290 | 0.3269 | 0.3116 | 0.1203 | 0.9214 | 0.8703 | 0.9242 |
| Jun27 | -0.0025 | -0.0009 | -0.0004 | 0.0012 | 0.3207 | 0.3059 | 0.1261 | 0.3232 | 0.3070 | 0.1249 | 0.9320 | 0.8803 | 0.9493 |
| Jun28 | -0.0020 | 0.0000 | -0.0010 | 0.0007 | 0.3240 | 0.3090 | 0.1275 | 0.3260 | 0.3090 | 0.1260 | 0.9266 | 0.8704 | 0.9345 |
| Jun28 | -0.0019 | -0.0006 | 0.0002 | 0.0019 | -9.9999 | -9.9999 | 0.1284 | -9.9900 | -9.9993 | 0.1265 | -0.0207 | -0.0207 | 0.9367 |
| Jul06 | -0.0002 | 0.0000 | 0.0003 | 0.0002 | 0.3140 | 0.2980 | 0.1220 | 0.3150 | 0.2980 | 0.1226 | 0.9620 | 0.9100 | 0.9619 |
| Jul07 | -0.0014 | 0.0010 | -0.0012 | 0.0007 | 0.3130 | 0.2985 | 0.1263 | 0.3152 | 0.2975 | 0.1256 | 0.9634 | 0.9093 | 0.9303 |
| Jul07 | -0.0012 | 0.0000 | -0.0001 | 0.0010 | 0.3105 | 0.2954 | 0.1225 | 0.3117 | 0.2954 | 0.1215 | 0.9703 | 0.9195 | 0.9700 |
| Jul09 | -0.0009 | 0.0013 | -0.0005 | 0.0007 | 0.3193 | 0.3039 | 0.1264 | 0.3202 | 0.3026 | 0.1257 | 0.9469 | 0.8940 | 0.9364 |
| Jul09 | -0.0025 | 0.0002 | -0.0011 | 0.0009 | 0.3130 | 0.2968 | 0.1255 | 0.3155 | 0.2986 | 0.1246 | 0.9595 | 0.9001 | 0.9447 |
| Jul10 | -0.0013 | 0.0010 | -0.0007 | 0.0006 | 0.3163 | 0.3016 | 0.1264 | 0.3176 | 0.3006 | 0.1250 | 0.9630 | 0.9020 | 0.9351 |
| Jul10 | -0.0021 | 0.0004 | -0.0007 | 0.0011 | 0.3119 | 0.2974 | 0.1146 | 0.3140 | 0.2970 | 0.1135 | 0.9645 | 0.9123 | 1.0364 |
| Jul11 | -0.0016 | 0.0000 | -0.0000 | 0.0006 | 0.3145 | 0.2994 | 0.1148 | 0.3161 | 0.2906 | 0.1142 | 0.9692 | 0.9061 | 1.0295 |
| Jul11 | -0.0026 | -0.0003 | -0.0005 | 0.0010 | 0.3060 | 0.2920 | 0.1116 | 0.3086 | 0.2931 | 0.1106 | 0.9772 | 0.9201 | 1.0630 |
| Jul20 | -0.0011 | 0.0007 | 0.0002 | 0.0007 | 0.3205 | 0.3061 | 0.1111 | 0.3216 | 0.3054 | 0.1104 | 0.9364 | 0.8892 | 1.0590 |
| Jul21 | -0.0003 | 0.0010 | 0.0005 | 0.0096 | 0.3224 | 0.3077 | 0.1142 | 0.3227 | 0.3067 | 0.1136 | 0.9323 | 0.8861 | 1.0206 |
| Jul21 | -0.0006 | 0.0020 | 0.0009 | 0.0010 | 0.3200 | 0.3061 | 0.1146 | 0.3214 | 0.3053 | 0.1136 | 0.9366 | 0.8896 | 1.0266 |
| Jul22 | -0.0007 | 0.0013 | 0.0005 | 0.0000 | 0.3229 | 0.3971 | 0.1175 | 0.3236 | 0.3050 | 0.1167 | 0.9349 | 0.8834 | 1.0006 |
| Jul22 | -0.0009 | 0.0004 | 0.0006 | 0.0012 | -9.9999 | -9.9999 | 0.1174 | -9.9990 | ******** | 0.1162 | -0.0206 | -0.0206 | 1.0049 |
| Jul24 | -0.0004 | 0.0013 | 0.0008 | 0.0007 | 0.3220 | 0.3071 | 0.1204 | 0.3224 | 0.3050 | 0.1197 | 0.9345 | 0.8864 | 0.9744 |
| Jul24 | -0.0033 | -0.0009 | 0.0003 | 0.0007 | 0.3130 | 0.2987 | 0.1155 | 0.3163 | 0.2996 | 0.1140 | 0.9539 | 0.9035 | 1.0160 |
| Jul25 | -0.0008 | 0.0009 | 0.0002 | 0.0006 | 0.3200 | 0.3053 | 0.1186 | 0.3200 | 0.3044 | 0.1100 | 0.9307 | 0.8907 | 0.9070 |
| Jul25 | -0.0019 | 0.0031 | 0.0005 | 0.0009 | -9.9999 | -9.9999 | 0.1160 | -9.9980 | ******** | 0.1151 | -0.0206 | -0.0206 | 1.0127 |
| Jul26 | -0.0010 | 0.0000 | 0.0005 | 0.0007 | -9.9999 | -9.9999 | 0.1188 | -9.9989 | ******** | 0.1101 | -0.0206 | -0.0206 | 0.9063 |
| Jul26 | -0.0016 | 0.0002 | 0.0005 | 0.0016 | 0.3100 | 0.3030 | 0.1173 | 0.3196 | 0.3020 | 0.1157 | 0.9435 | 0.8939 | 1.0060 |
| Jul28 | 0.0010 | 0.0012 | 0.0010 | -0.0021 | 0.3219 | 0.3066 | 0.1168 | 0.3209 | 0.3054 | 0.1109 | 0.9351 | 0.8900 | 0.9765 |
| Jul28 | 0.0023 | 0.0012 | 0.0034 | -0.0000 | 0.3237 | 0.3079 | 0.1163 | 0.3214 | 0.3067 | 0.1171 | 0.9312 | 0.8806 | 0.9935 |
| Jul29 | 0.0000 | 0.0017 | 0.0005 | -0.0011 | 0.3239 | 0.3094 | 0.1189 | 0.3239 | 0.3077 | 0.1200 | 0.9200 | 0.8816 | 0.9609 |
| Jul29 | -0.0003 | 0.0013 | 0.0060 | -0.0014 | 0.3244 | 0.3093 | 0.1103 | 0.3247 | 0.3000 | 0.1197 | 0.9271 | 0.8794 | 0.9714 |
| Jul31 | 0.0001 | 0.0000 | 0.0016 | 0.0006 | 0.3193 | 0.3010 | 0.1210 | 0.3192 | 0.3032 | 0.1212 | 0.9414 | 0.8942 | 0.9592 |
| Aug02 | -0.0030 | -0.0005 | 0.0000 | 0.0006 | 0.3424 | 0.3164 | 0.1212 | 0.3454 | 0.3169 | 0.1206 | 0.9064 | 0.8261 | 0.9617 |
| Aug02 | -0.0021 | -0.0010 | 0.0000 | 0.0013 | 0.3342 | 0.3155 | 0.1200 | 0.3363 | 0.3165 | 0.1107 | 0.9016 | 0.8495 | 0.9771 |
| Aug03 | -0.0010 | 0.0042 | 0.0004 | 0.0007 | 0.3249 | 0.3082 | 0.1210 | 0.3267 | 0.3000 | 0.1211 | 0.9263 | 0.8733 | 0.9572 |
| Aug03 | -0.0030 | -0.0009 | 0.0004 | 0.0009 | 0.3163 | 0.3014 | 0.1107 | 0.3193 | 0.3023 | 0.1170 | 0.9437 | 0.8935 | 0.9810 |
| Aug04 | -0.0042 | -0.0020 | 0.0002 | 0.0007 | 0.3160 | 0.2999 | 0.1161 | 0.3200 | 0.3019 | 0.1154 | 0.9440 | 0.8914 | 1.0030 |
| Aug04 | -0.0032 | -0.0069 | 0.0003 | 0.0000 | -9.9999 | -9.9999 | 0.1172 | -9.9967 | -9.9990 | 0.1164 | -0.0205 | -0.0205 | 0.9962 |
| Aug05 | -0.0039 | -0.0023 | 0.0000 | 0.0000 | -9.9999 | -9.9999 | 0.1126 | -9.9960 | -9.9976 | 0.1110 | -0.0205 | -0.0285 | 1.0355 |
| Aug05 | -0.0034 | -0.0012 | 0.0005 | 0.0009 | 0.3153 | 0.3012 | 0.1144 | 0.3107 | 0.3024 | 0.1135 | 0.9431 | 0.8949 | 1.0260 |
| Aug06 | -0.0042 | -0.0021 | 0.0007 | 0.0007 | 0.3141 | 0.2991 | 0.1090 | 0.3103 | 0.3012 | 0.1009 | 0.9467 | 0.8950 | 1.0624 |
| Aug06 | -0.0040 | -0.0020 | 0.0004 | 0.0000 | 0.3122 | 0.2982 | 0.1162 | 0.3162 | 0.3002 | 0.1154 | 0.9499 | 0.9010 | 1.0026 |
| Aug07 | -0.0057 | -0.0031 | 0.0006 | 0.0007 | 0.3101 | 0.2960 | 0.1140 | 0.3150 | 0.2991 | 0.1141 | 0.9532 | 0.9020 | 1.0134 |
| Aug07 | -0.0034 | -0.0010 | 0.0004 | 0.0015 | 0.3111 | 0.2975 | 0.1172 | 0.3145 | 0.2993 | 0.1157 | 0.9525 | 0.9065 | 0.9994 |
| Aug08 | -0.0062 | -0.0036 | 0.0004 | 0.0007 | 0.3006 | 0.2950 | 0.1164 | 0.3140 | 0.2986 | 0.1157 | 0.9546 | 0.9055 | 0.9987 |
| Aug08 | -0.0030 | -0.0021 | 0.0003 | 0.0000 | 0.3111 | 0.2973 | 0.1101 | 0.3149 | 0.2994 | 0.1173 | 0.9521 | 0.9052 | 0.9851 |
| Aug16 | -0.0000 | 0.0001 | 0.0015 | 0.0006 | 0.3230 | 0.3071 | 0.1293 | 0.3230 | 0.3070 | 0.1197 | 0.9272 | 0.8791 | 0.9606 |

## Table 11, cont. NOX AND O3 CALIBRATIONS FOR 1984

16-May-1986

| DATE | NOX ZERO | NO ZERO | NO2 ZERO | O3 ZERO | NOX SPAN | NO SPAN | O3 SPAN | NOX RESP | NO RESP | O3 RESP | NO CAL | NOX CAL | O3 CAL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Aug18 | -0.0040 | -0.0027 | 0.0011 | 0.0007 | 0.3164 | 0.3019 | 0.1167 | 0.3204 | 0.3046 | 0.1160 | 0.9342 | 0.8881 | 0.9903 |
| Aug18 | -0.0045 | -0.0025 | 0.0004 | 0.0007 | 0.3172 | 0.2999 | 0.1162 | 0.3217 | 0.3024 | 0.1155 | 0.9410 | 0.8845 | 0.9943 |
| Aug19 | -0.0047 | -0.0027 | 0.0002 | 0.0000 | 0.3140 | 0.2999 | 0.1175 | 0.3187 | 0.3026 | 0.1167 | 0.9402 | 0.8927 | 0.9834 |
| Aug19 | -0.0035 | -0.0020 | 0.0009 | 0.0015 | 0.3139 | 0.2986 | 0.1183 | 0.3174 | 0.3006 | 0.1168 | 0.9465 | 0.8964 | 0.9826 |
| Aug20 | -0.0040 | -0.0027 | 0.0006 | 0.0000 | 0.3140 | 0.3002 | 0.1192 | 0.3196 | 0.3029 | 0.1184 | 0.9391 | 0.8981 | 0.9667 |
| Aug20 | -0.0047 | -0.0031 | 0.0010 | 0.0010 | 0.3147 | 0.3004 | 0.1166 | 0.3194 | 0.3035 | 0.1175 | 0.9373 | 0.8906 | 0.9761 |
| Aug22 | -0.0045 | -0.0034 | 0.0014 | 0.0000 | 0.3183 | 0.3037 | 0.1200 | 0.3220 | 0.3071 | 0.1200 | 0.9260 | 0.8889 | 0.9546 |
| Aug22 | -0.0012 | -0.0023 | 0.0030 | 0.0000 | 0.3209 | 0.3049 | 0.1201 | 0.3221 | 0.3072 | 0.1193 | 0.9257 | 0.8820 | 0.9602 |
| Aug23 | -0.0036 | -0.0026 | 0.0016 | 0.0000 | 0.3197 | 0.3044 | 0.1265 | 0.3233 | 0.3070 | 0.1257 | 0.9261 | 0.8794 | 0.9187 |
| Aug25 | 0.0050 | 0.0000 | 0.0060 | 0.0010 | 0.3140 | 0.2945 | 0.1215 | 0.3090 | 0.2945 | 0.1205 | 0.9651 | 0.9198 | 0.9460 |
| Aug25 | 0.0020 | -0.0010 | 0.0050 | 0.0010 | 0.3155 | 0.2965 | 0.1250 | 0.3135 | 0.2976 | 0.1240 | 0.9553 | 0.9066 | 0.9220 |
| Aug27 | 0.0016 | -0.0014 | 0.0044 | 0.0023 | 0.3166 | 0.2992 | 0.1255 | 0.3149 | 0.3006 | 0.1232 | 0.9452 | 0.9022 | 0.9269 |
| Aug28 | -0.0010 | -0.0010 | 0.0031 | 0.0000 | 0.3144 | 0.2983 | 0.1246 | 0.3154 | 0.3001 | 0.1240 | 0.9466 | 0.9007 | 0.9263 |
| Aug29 | -0.0022 | -0.0026 | 0.0026 | 0.0000 | 0.3143 | 0.2980 | 0.1246 | 0.3165 | 0.3006 | 0.1230 | 0.9440 | 0.8974 | 0.9212 |
| Aug29 | -0.0007 | -0.0010 | 0.0027 | 0.0000 | 0.3129 | 0.2972 | 0.1185 | 0.3136 | 0.2990 | 0.1177 | 0.9499 | 0.9057 | 0.9694 |
| Sep01 | -0.0014 | -0.0022 | 0.0031 | 0.0017 | 0.3153 | 0.2997 | 0.1172 | 0.3167 | 0.3019 | 0.1155 | 0.9403 | 0.8963 | 0.9856 |
| Sep01 | -0.0014 | -0.0022 | 0.0031 | 0.0017 | 0.7439 | 0.7060 | 0.1172 | 0.7453 | 0.7002 | 0.1155 | 0.9309 | 0.8957 | 0.9856 |
| Sep02 | -0.0020 | -0.0020 | 0.0020 | 0.0000 | 0.7377 | 0.6920 | 0.1172 | 0.7405 | 0.6940 | 0.1164 | 0.9563 | 0.9009 | 0.9773 |
| Sep02 | -0.0037 | -0.0031 | 0.0010 | 0.0007 | 0.7377 | 0.6920 | 0.1172 | 0.7414 | 0.6961 | 0.1165 | 0.9559 | 0.8998 | 0.9765 |
| Sep02 | -0.0027 | -0.0025 | 0.0019 | 0.0007 | 0.7269 | 0.6813 | 0.1189 | 0.7296 | 0.6830 | 0.1182 | 0.9717 | 0.9144 | 0.9624 |
| Sep03 | -0.0042 | -0.0021 | -0.0001 | 0.0009 | 0.7390 | 0.6949 | 0.1173 | 0.7432 | 0.6970 | 0.1164 | 0.9526 | 0.8970 | 0.9767 |
| Sep06 | 0.0055 | 0.0003 | 0.0073 | 0.0000 | 0.7447 | 0.6969 | 0.1193 | 0.7392 | 0.6966 | 0.1185 | 0.9511 | 0.9000 | 0.9576 |
| Sep06 | 0.0061 | 0.0017 | -9.9999 | 0.0022 | 0.7447 | 0.6969 | 0.1197 | 0.7306 | 0.6952 | 0.1171 | 0.9530 | 0.9007 | 0.9650 |
| Sep08 | 0.0047 | 0.0055 | 0.0059 | -9.9999 | 0.7590 | 0.7140 | 0.1192 | 0.7543 | 0.7135 | ******** | 0.9273 | 0.8807 | 0.0112 |
| Sep08 | -0.0016 | -0.0013 | 0.0015 | 0.0021 | 0.7601 | 0.7149 | 0.1135 | 0.7617 | 0.7162 | 0.1118 | 0.9230 | 0.8722 | 1.0137 |
| Sep09 | -0.0016 | -0.0036 | 0.0009 | 0.0007 | 0.7626 | 0.7196 | 0.1194 | 0.7642 | 0.7202 | 0.1107 | 0.9180 | 0.8607 | 0.9541 |
| Sep09 | -0.0027 | -0.0014 | 0.0006 | 0.0010 | 0.7536 | 0.7092 | 0.1155 | 0.7563 | 0.7106 | 0.1145 | 0.9304 | 0.8770 | 0.9891 |
| Sep16 | -0.0033 | -0.0023 | 0.0011 | 0.0031 | 0.7500 | 0.7010 | 0.1270 | 0.7533 | 0.7033 | 0.1239 | 0.9354 | 0.8769 | 0.9130 |
| Sep16 | -0.0047 | -0.0029 | 0.0004 | 0.0013 | 0.7529 | 0.7026 | 0.1258 | 0.7576 | 0.7054 | 0.1245 | 0.9326 | 0.8719 | 0.9057 |
| Sep17 | -0.0030 | -0.0023 | 0.0002 | 0.0007 | 0.7501 | 0.7003 | 0.1270 | 0.7619 | 0.7106 | 0.1271 | 0.9252 | 0.8664 | 0.8866 |
| Sep17 | -0.0042 | -0.0030 | 0.0009 | 0.0011 | 0.7506 | 0.6996 | 0.1266 | 0.7547 | 0.7026 | 0.1256 | 0.9350 | 0.8747 | 0.8979 |
| Sep18 | -0.0037 | -0.0026 | 0.0005 | 0.0000 | 0.7541 | 0.7050 | 0.1275 | 0.7570 | 0.7076 | 0.1267 | 0.9204 | 0.8705 | 0.8880 |
| Sep18 | -0.0044 | -0.0032 | 0.0010 | 0.0000 | 0.7479 | 0.6970 | 0.1260 | 0.7523 | 0.7002 | 0.1250 | 0.9302 | 0.8760 | 0.9069 |
| Sep19 | -0.0040 | -0.0031 | 0.0005 | 0.0007 | 0.7552 | 0.7040 | 0.1269 | 0.7592 | 0.7071 | 0.1262 | 0.9204 | 0.8603 | 0.8910 |
| Sep19 | -0.0030 | -0.0031 | 0.0020 | 0.0014 | 0.7453 | 0.6930 | 0.1213 | 0.7403 | 0.6961 | 0.1199 | 0.9431 | 0.8809 | 0.9366 |
| Sep21 | -0.0052 | -0.0034 | 0.0006 | 0.0000 | 0.7316 | 0.6771 | 0.1107 | 0.7367 | 0.6806 | 0.1179 | 0.9633 | 0.8935 | 0.9533 |
| Sep21 | -0.0027 | -0.0025 | 0.0022 | 0.0019 | 0.7273 | 0.6706 | 0.1103 | 0.7300 | 0.6731 | 0.1164 | 0.9739 | 0.9017 | 0.9656 |
| Sep25 | -0.0052 | -0.0036 | 0.0002 | 0.0007 | 0.7271 | 0.6710 | 0.1166 | 0.7323 | 0.6754 | 0.1150 | 0.9670 | 0.8963 | 0.9681 |
| Sep25 | -0.0001 | -0.0030 | 0.0014 | 0.0009 | -9.9999 | 0.6691 | 0.1181 | -9.9990 | 0.6729 | 0.1172 | 0.9714 | -0.0656 | 0.9566 |
| Oct03 | -0.0020 | -0.0020 | 0.0020 | 0.0000 | -9.9999 | -9.9999 | -9.9999 | -9.9971 | -9.9971 | ******** | -0.0650 | -0.0653 | -0.0112 |
| Oct05 | -0.0037 | -0.0033 | 0.0020 | 0.0000 | 0.7290 | 0.6742 | 0.1122 | 0.7327 | 0.6776 | 0.1114 | 0.9679 | 0.8894 | 0.9999 |
| Oct05 | -0.0036 | -0.0041 | 0.0026 | 0.0007 | 0.7267 | 0.6723 | 0.1109 | 0.7293 | 0.6764 | 0.1102 | 0.9595 | 0.8936 | 1.0100 |
| Oct06 | -0.0050 | -0.0046 | 0.0019 | 0.0007 | 0.7306 | 0.6760 | 0.1113 | 0.7356 | 0.6806 | 0.1106 | 0.9529 | 0.8853 | 1.0065 |
| Oct06 | -9.9999 | -9.9999 | -9.9999 | -9.9999 | 0.7396 | 0.6872 | 0.1063 | ******** | ******** | ******** | 0.0607 | 0.8606 | 0.0110 |
| Oct07 | -0.0054 | -0.0045 | 0.0011 | 0.0007 | 0.7420 | 0.6904 | 0.1076 | 0.7474 | 0.6949 | 0.1069 | 0.9326 | 0.8707 | 1.0407 |
| Oct07 | -0.0054 | -0.0065 | 0.0019 | 0.0009 | 0.7414 | 0.6881 | 0.1073 | 0.7460 | 0.6946 | 0.1064 | 0.9330 | 0.8714 | 1.0456 |
| Oct09 | -0.0040 | -0.0043 | 0.0010 | 0.0007 | 0.7440 | 0.6910 | 0.1074 | 0.7496 | 0.6953 | 0.1067 | 0.9307 | 0.8669 | 1.0413 |
| Oct10 | -0.0046 | -0.0055 | 0.0025 | 0.0020 | 0.7400 | 0.6858 | 0.1075 | 0.7445 | 0.6906 | 0.1055 | 0.9365 | 0.8722 | 1.0524 |
| Oct11 | -0.0051 | -0.0040 | 0.0019 | 0.0007 | 0.7364 | 0.6834 | 0.1061 | 0.7415 | 0.6802 | 0.1054 | 0.9309 | 0.8751 | 1.0520 |

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**Table 11, cont.** NOX AND O3 CALIBRATIONS FOR 1984

16-May-1986

| DATE | NOX ZERO | NO ZERO | NO2 ZERO | O3 ZERO | NOX SPAN | NO SPAN | O3 SPAN | NOX RESP | NO RESP | O3 RESP | NO CAL | NOX CAL | O3 CAL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Oct11 | -0.0050 | -0.0044 | 0.0021 | 0.0022 | 0.7352 | 0.6833 | 0.1140 | 0.7402 | 0.6877 | 0.1110 | 0.9396 | 0.8766 | 0.9925 |
| Oct12 | -0.0060 | -0.0046 | 0.0010 | 0.0000 | 0.7372 | 0.6843 | 0.1134 | 0.7432 | 0.6809 | 0.1126 | 0.9373 | 0.8725 | 0.9840 |
| Oct12 | -0.0041 | -0.0048 | 0.0027 | 0.0000 | 0.7354 | 0.6813 | 0.1119 | 0.7395 | 0.6861 | 0.1111 | 0.9411 | 0.8760 | 0.9981 |
| Oct13 | -0.0035 | -0.0039 | 0.0024 | 0.0000 | 0.7413 | 0.6896 | 0.1137 | 0.7440 | 0.6935 | 0.1129 | 0.9304 | 0.8700 | 0.9816 |
| Oct13 | -0.0042 | -0.0046 | 0.0029 | 0.0000 | 0.7344 | 0.6807 | 0.1135 | 0.7386 | 0.6853 | 0.1127 | 0.9415 | 0.8773 | 0.9833 |
| Oct14 | -0.0029 | -0.0033 | 0.0029 | 0.0000 | 0.7409 | 0.6873 | 0.1130 | 0.7430 | 0.6906 | 0.1122 | 0.9336 | 0.8705 | 0.9870 |
| Oct14 | -0.0043 | -0.0046 | 0.0028 | 0.0007 | 0.7349 | 0.6806 | 0.1135 | 0.7392 | 0.6852 | 0.1120 | 0.9410 | 0.8759 | 0.9810 |
| Oct15 | -0.0031 | -0.0030 | 0.0027 | 0.0010 | 0.7560 | 0.7020 | 0.1155 | 0.7591 | 0.7050 | 0.1145 | 0.9139 | 0.8523 | 0.9666 |
| Oct23 | -0.0087 | -0.0074 | 0.0018 | 0.0007 | 0.6837 | 0.6344 | 0.1100 | 0.6924 | 0.6410 | 0.1101 | 0.9901 | 0.9290 | 0.9322 |
| Oct25 | -0.0091 | -0.0073 | 0.0000 | 0.0006 | -9.9999 | -9.9999 | 0.1147 | -9.9900 | -9.9926 | 0.1141 | -0.0640 | -0.0643 | 0.9637 |
| Oct26 | -0.0053 | -0.0055 | -0.0026 | 0.0010 | 0.6980 | 0.6456 | 0.1200 | 0.7033 | 0.6510 | 0.1190 | 0.9025 | 0.9133 | 0.9240 |

Figure 9 shows the flowchart for HC calibration data processing with CALENTRY events indicated. Table 12 shows the RUNENTRY events flowchart.

### *Identification of Calibration Chromatogram and Calibration Source*

If one or more forms of documentation indicate that a calibration(s) was performed, then the first step is to identify the data and calibration source(s). If the calibration was performed during an experiment, it was logged in CALENTRY when the experiment was logged in RUNENTRY. Otherwise, the run calendars indicate a calibration event and the presence of a new calibration folder. If the calibration occured during an experiment, the run folder INSTRUMENT INVENTORY CHECKLIST indicates the instruments calibrated, otherwise, the stripcharts present in the calibration folder indicate which instruments were calibrated. Calibration sources are identified on the stripcharts.

### *Issue Calibration Pick Instructions*

Calibration processing (pick) instructions are given by the PC via the CAL PICK INSTRUCTION form. The form is stored in the CAL PICK INSTRUCTION NOTEBOOK by date. The fact that pick instructions are given is entered into CALENTRY. Several QA steps occur at this point. Documentation is checked for reasonableness and completeness (sources, chart settings, instrument settings). The chromatograms are inspected for reasonableness (match standard example chromatograms with source for conditions specified).

### *Official Calibration Sources/ OCS Report*

The raw data can be processed (picked), but before final processing can occur, the calibration source data must be validated and entered into the OFFICIAL CALIBRATION SOURCE (OCS) DATATRIEVE database and the OCSFIL.DAT updated. The forms used for recording the OCS data were discussed above.

Several sources are used throughout the season. These were listed above. The validation procedure was also reported. The first step is to check the report from the OCS database to see if the source has been entered. If the OCS does not exist then it must be created or at least validated. The details of processing single (used once) OCS are discussed next. The OCS report is listed in Appendix C.

### *Create OCS for Single Injection*

These OCS are created in the smog chamber. The amounts of HC that are injected are documented along with the chamber temperature in the calibration folders or on the RUN SHEET. A LOTUS 123 database/spreadsheet OCSIC (described above) is used

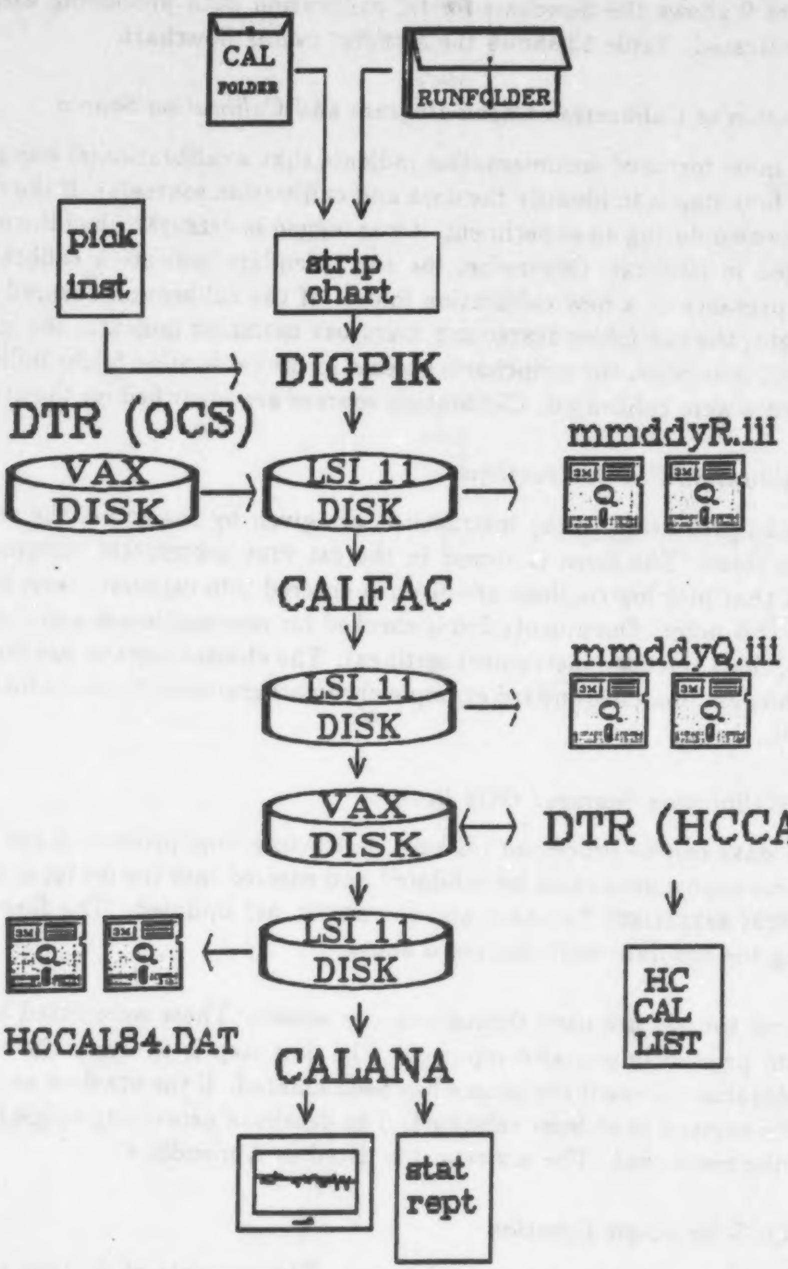

CAL
FOLDER
RUNFOLDER
pick
inst
strip
chart
DIGPIK
DTR (OCS)
VAX
DISK
LSI 11
DISK
mmddyR.iii
CALFAC
LSI 11
DISK
mmddyQ.iii
VAX
DISK
DTR (HCCAL)
LSI 11
DISK
HCCAL84.DAT
HC
CAL
LIST
CALANA
stat
rept

**Figure 9. HC Autocal Processing Flowchart.**

# Table 12.

## Processing System for Instrument Auto-Calibration Data

```
   tot inst    cal analysis
          \   /           \
          !CPI!           !OCS!
             \               \
              \               \
               <DPR>----------<CFR>--(Q2V)--(DTR)--(C2L)--<CLR>--!CQA!
```

```
      !sss! == stages determined by Project coordinator (PC)
      <sss> == stages determined by Peak Pickers (PP)
      (sss) == stages determined by Computer Techs (CT)
```

| Step | CALENTRY stages | Meaning |
|---|---|---|
| PC | CPI : CAL pick Inst | Charts marked, cal status sheet in folder |
| PP | DPR : Digpik run | Cal data digitized and R-file exists |
| PC | OCS : OCS ok | Official Cal Source exists in DTR |
| PP | CFR : CALFAC run | Cal Factor computed, Q-file created |
| CT | Q2V : Qfile to vax | Q-file moved to VAX |
| CT | DTR : DTR file updated | Cal Data added to DTR data base |
| CT | C2L : Cals to LSI | DTR CAL file loaded on LSI-11 |
| PP | CLR : CALANA run | Cal Factors analyzed |
| PC | CQA : Cal QA | Cal Factor Quality Assurance |
| PC | NTB : Not to be proc | Not to be processed |
| PC | BAD : Stop processing | Something is wrong with this run |

to process this information. The species id number is used to look up all the necessary species specific information (density, molecular weight, carbon number, *etc.*) and the program calculates and records the ideal concentration. Table 4 lists the OCSIC report. All OCS information is recorded on OCS forms and recorded in the OCS notebook as described above. The validated OCS concentrations are entered into the DATATRIEVE database CAL_SOURCES_FNS. A database report procedure is used to update the OCSFIL.DAT which is transfered to the LSI to await final processing. The fact that the OCS exists is entered into the DATATRIEVE CALENTRY database.

### *Run DIGPIK on calibration Data to Make R-files*

Once calibration processing instructions have been given, raw data are picked using a program on the LSI (DIGPIK) where the data are digitized and a response file (`R-file`, `MMDDYR.iit`) is produced. The files are backed-up (copied) onto floppies.

### *Run CALFAC to Calculate Calibration Factors*

Once the response data has been picked and the OCS data has been updated to OCSFIL.DAT, the calibration factor can be calculated. A program on the LSI CALFAC is run which reads the internal documentation in the response file `R-file` and compares the data with the appropriate OCS to generate the concentration per response unit calibration factor. A QA step is performed here. The calibration factors are inspected and reviewed in context with the existing database with the program CALLOK which plots or lists the data vs. julian date with a linear least-squares fit. The program identifies calibration data which varies by more than a specified percentage. The generated calibration data is output in files ("Q"-files) specific for the instrument and the day calibrated. These files are backed-up on floppy.

The Q-files are transferred and updated to the DATATRIEVE HC_CAL database if the calibration data seems reasonable. A DATATRIEVE report procedure PRINT_HC_CAL_FACTORS, is run to generate an updated calibration list sorted by instrument, species, and date. All data are converted to a single specified attenuation for easy inspection. Another DATATRIEVE procedure, PRINT_FILE_CALANA, is used to generate another file which is then transfered to the LSI-11/23 computer to be used by a program called CALANA which performs a statistical and graphical analysis of the calibration database.

We expect a certain amount of noise or variation based on experience. Usually the calibration factors are very stable with little or no trend demonstrated. Variations are found, however, and some are real indications of instrument change. Discrepancies that are more than a few percent are investigated. Figure 10 shows example CALANA plots and statistical reports. Appendix D contains a larger collection of these plots and statistics.

The statistical report first lists the data range searched in the database. The number of data points found and included for the analysis are listed. The slope and intercept of the straight line fit through the data are listed with the standard deviation and relative standard deviation. The correlation coefficient is also listed. The minimum, maximum and mean of the data are shown with the standard deviation and relative standard deviation. Lastly the equation of the straight line fit is shown. Table 13 shows a compilation of the statistics from this set.

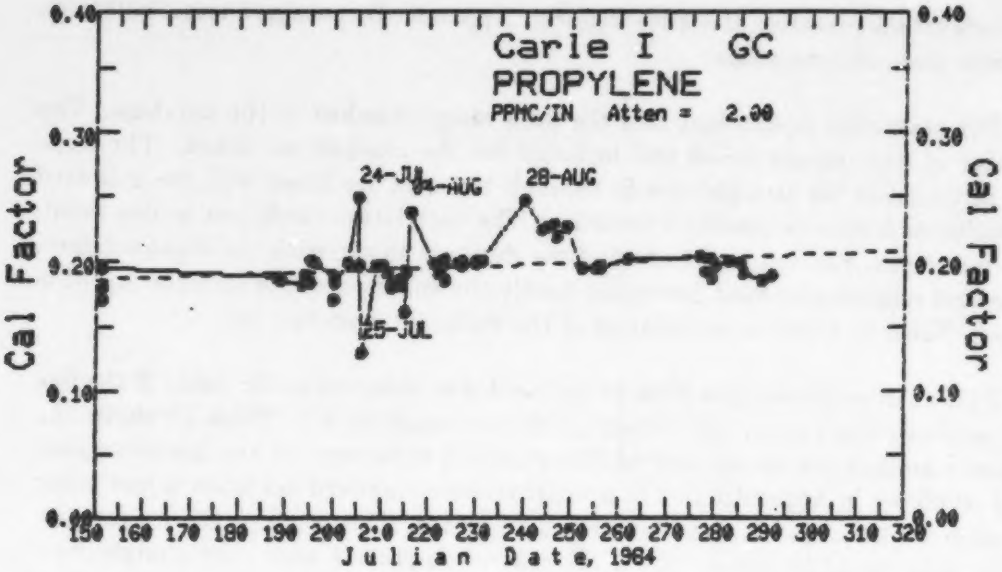
This analysis shows that little or no trend was observed in the data. If the line was perfectly horizontal, the correlation factor would be 0.0. Table 13 shows the means, standard deviations, and relative standard deviations for the more complete data set shown in Appendix D. The average relative standard deviation is just under 10 percent with a standard deviation of 2.2 percent. This suggests the uncertainty in the data would be about 10% *if the calibration factors were used straight from the initial processing and no additional information and QA techniques were used to check and tune the calibration data.* Because specific calibration factors are used and because the data are subjected to further examination and adjustment, the uncertainty in the final data is less than 10%.

Valid deviations can be caused by many factors. including variation in the instrument operating characteristics. Calibration factors specific to the current instrument status should be used rather than some average value. Non-valid sources of calibration data deviation include improper processing. Many QA measures are taken to prevent these errors. These measures will be discussed further.

There are several explanations for variation in calibration data. Insufficient sample flow will result in very low responses and consequently very large calibration factors. Sometimes the instrument operating conditions change (*e.g.* carrier flow) which changes the peak width and consequently the calibration factor. Incorrectly recorded attenuation will, of course, cause generated calibration data to be off by a factor of multiples of 2 or 10. The Perkin Elmer Sigma 10 integrator which yields areas not affected by the GC attenuation settings, can be compared with areas of calibrations performed on other days to determine if this type of problem has occurred; the attenuation can be corrected in the "R" file and reprocessed.

### *Estimation of Calibration Factors for Infrequently Calibrated* HC

The technique discussed above requires an explicit calibration source for the com-



```
For the species PROPYLENE and the instrument Carle I   GC:

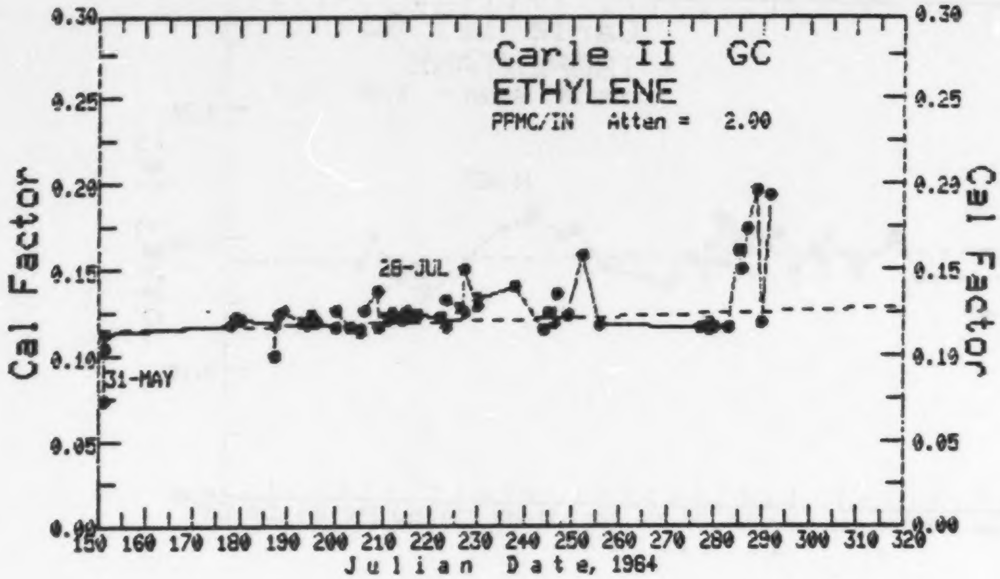
Beginning Caldate:          30-MAY-84
                      Day:  150
Ending    Caldate:          16-NOV-84
                      Day:  320
Upper CalFactor Limit         0.40000
Lower CalFactor Limit         0.00000

The number of data points     62
The number included  was      62
The slope of this fit  is 1.3522654E-004
      with a std dev of 6.6911662E-005   rel. dev = 49.5 %
The intercept is          1.6694184E-001
      with a std dev of 1.5341250E-002   rel. dev = 9.2 %
The std dev of the fit is 1.8079919E-002   PE =  0.01205
The correlation coeff is   0.25246

The min, mean, max are        0.13040,    0.19760,    0.25009
The standard deviation is  0.01853   rel. dev = 9.4 %

Cal =  0.00014 X (Julian Date - 150) +  0.18723
```

**Figure 10.** CALANA Example Figures.



```
For the species ETHYLENE and the instrument Carle II  GC:

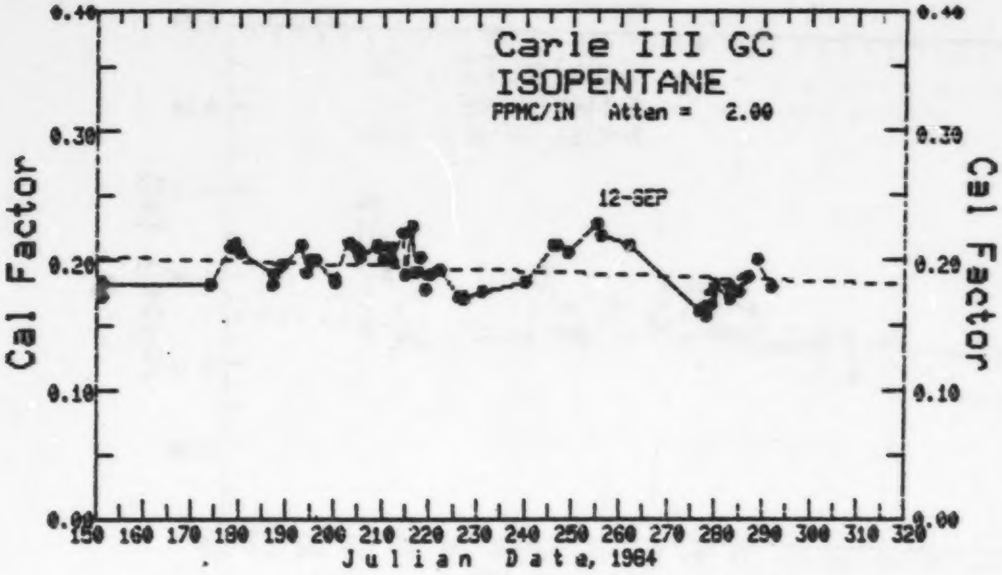
Beginning Caldate:           30-MAY-84
                       Day:  150
Ending    Caldate:           16-NOV-84
                       Day:  320
Upper CalFactor Limit            0.14000
Lower CalFactor Limit            0.00000

The number of data points        61
The number included  was         53
The slope of this fit  is 7.7424523E-005
       with a std dev of 3.6302085E-005   rel. dev = 46.9 %
The intercept is          1.0432247E-001
       with a std dev of 7.9898236E-003   rel. dev = 7.7 %
The std dev of the fit is 8.8857276E-003   PE =  0.00592
The correlation coeff is   0.28616

The min, mean, max are        0.07444,    0.12116,    0.19795
The standard deviation is  0.00918   rel. dev = 7.6 %

Cal =  0.00008 X (Julian Date - 150) +  0.11594
```

**Figure 10, cont. CALANA Example Figures.**



```
For the species ISOPENTANE and the instrument Carle III GC:

Beginning Caldate:          30-MAY-84
                      Day:  150
Ending    Caldate:          16-NOV-84
                      Day:  320
Upper CalFactor Limit          0.40000
Lower CalFactor Limit          0.00000

The number of data points     60
The number included  was      60
The slope of this fit  is -1.222656E-004
       with a std dev of 5.6003271E-005   rel. dev = -45.8 %
The intercept is          2.2209272E-001
       with a std dev of 1.2738738E-002   rel. dev = 5.7 %
The std dev of the fit is 1.6698649E-002   PE =  0.01113
The correlation coeff is  -0.27557

The min, mean, max are       0.15986,    0.19468,    0.23074
The standard deviation is  0.01722   rel. dev = 8.8 %

Cal = -0.00012 X (Julian Date - 150) +  0.20375
```

**Figure 10, cont.** CALANA Example Figures.

**Table 13.** Summary of CALANA Statistics

| | | MIN | MAX | MEAN | STD DEV | REL STD DEV |
|---|---|---|---|---|---|---|
| Carle I | | | | | | |
| | propylene | 0.130 | 0.250 | 0.198 | 0.019 | 9.4% |
| | isopentane | 0.140 | 0.196 | 0.158 | 0.010 | 6.3% |
| Carle II | | | | | | |
| | ethylene | 0.074 | 0.193 | 0.121 | 0.009 | 7.6% |
| | ethane | 0.013 | 0.231 | 0.147 | 0.007 | 5.0% |
| | propylene | 0.369 | 0.976 | 0.553 | 0.054 | 9.8% |
| | propane | 0.428 | 1.059 | 0.607 | 0.060 | 9.9% |
| Carle III | | | | | | |
| | 1-butene | 0.074 | 0.130 | 0.100 | 0.011 | 11.5% |
| | n-butane | 0.053 | 0.131 | 0.102 | 0.016 | 11.7% |
| | cis-2-butene | 0.070 | 0.127 | 0.105 | 0.015 | 14.0% |
| | trans-2-butene | 0.091 | 0.132 | 0.115 | 0.011 | 9.2% |
| | 1,3-butadiene | 0.090 | 0.137 | 0.116 | 0.012 | 9.9% |
| | isopentane | 0.160 | 0.231 | 0.195 | 0.017 | 8.8% |
| | n-pentane | 0.228 | 0.347 | 0.289 | 0.028 | 9.8% |
| | benzene | 0.080 | 0.106 | 0.090 | 0.009 | 10.3% |
| | toluene | 0.114 | 0.167 | 0.137 | 0.014 | 10.0% |
| | m-xylene | 0.187 | 0.269 | 0.225 | 0.027 | 12.0% |
| | o-xylene | 0.256 | 0.318 | 0.281 | 0.024 | 8.7% |
| | methanol | 0.835 | 1.206 | 1.050 | 0.143 | 13.7% |
| | ave | | | | | 9.9% |
| | std dev | | | | | 2.2% |

pound being monitored to generate a calibration factor. Sometimes calibration data is sparse or the species to be processed has no explicit calibration source. There are several techniques for establishing appropriate calibration factors. These are often used together.

When sufficient supporting calibration data exists, a plot of the calibration factors of well calibrated compounds measured on the same column, as a function of retention time, can be least-squares fit to an exponential function. A LOTUS 123 spreadsheet called CALEXTR is used for this. Figure 11 shows plots for the two columns in the Carle III GC. Our experience has been that good fits are obtained. The calibration factor for the uncalibrated compound can be estimated by locating its retention time on the curve. The ratios of the frequently calibrated compounds to the less frequently calibrated compounds can be determined for future needs. If integrator data is available, a check is done using integrator areas ratioed to the estimated concentrations of all the compounds.

If the compound requiring a calibration factor is part of a well characterized mixture (the source), the concentrations of the other compounds can be used to determine the concentration of the compound in question by ratios. The calibration factor can then be calculated.

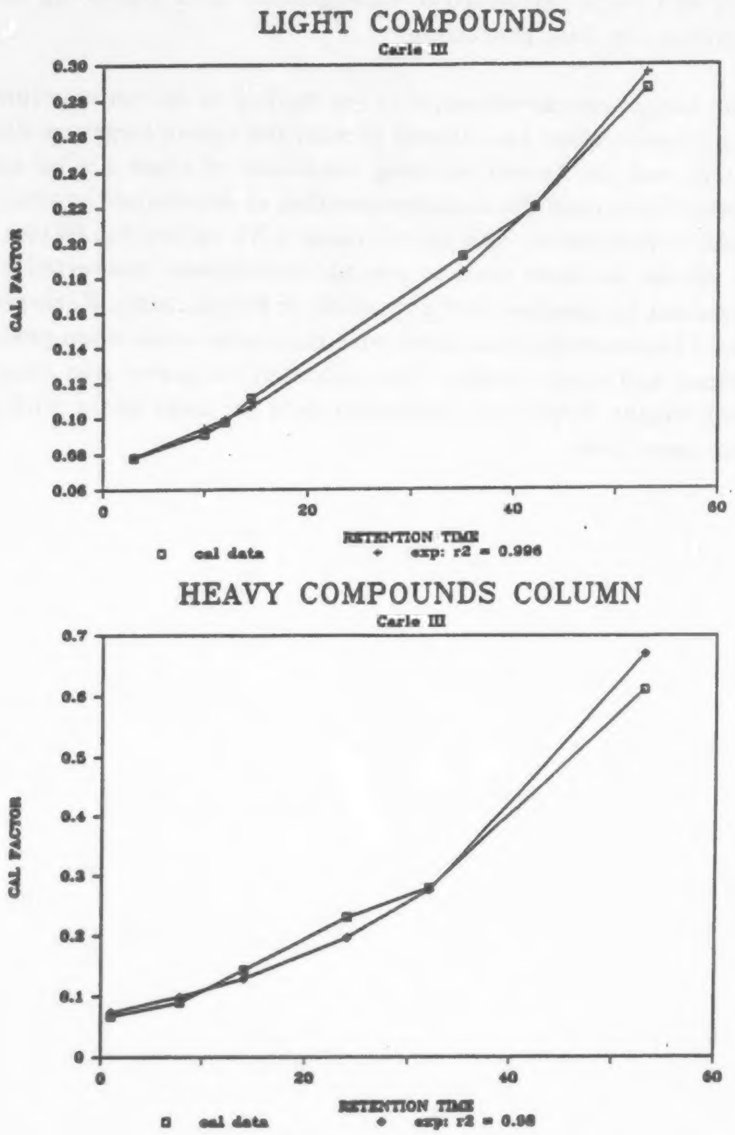
If reliable integrator data is available, the area count can be calibrated with any known calibration sources, and the corrected area used to determine the concentration of the uncalibrated compound. The concentration can then be used to calculate the calibration factor for the picked data.

If good calibration data exists for all species at some time, ratios of less frequently calibrated species to frequently calibrated species can be determined. These ratios can be used to calculate calibration factors for times when the calibration data are less complete.

### *Final Calibration Factor Calculations*

To process data, calibration factors can be taken from the HCCAL DATATRIEVE report for explicit calibrations or extrapolated from calibration data for other species. Calibrations may not have been performed the day of an experiment for all species. Interpolation may be needed between the calibrations for a species done right before and after the day in question.

The discussion to this point has been concerned with the processing of calibration data and using calibration data to estimate calibration factors for compounds



LIGHT COMPOUNDS

Carle III

HEAVY COMPOUNDS COLUMN

Carle III

**Figure 11.** Calextr Examples.

not explicitly calibrated. Calibration factors need additional checking and perhaps adjustment sometimes before they are applied to process data. These checking procedures are actually QA steps performed in experimental data processing but are definitely part of calibration data processing.

Once calibration factors are calculated, they are applied to the raw experimental data. The resulting concentration data should fit with the known target conditions, the amounts injected, and the known resulting conditions of other similar experiments. The data should also yield the same composition as determined by analytical data for other similar experiments. This should occur with calibration factors used which are at least similar to those used to process experiments conducted before and after the experiment in question (see discussion of `RUN_CAL_USED`). Ratios of initial conditions should be somewhat consistent with integrator areas when peaks are reasonably well defined and integrateable. The calibrated integrator area should be consistent with peak height derived concentration data for large peaks with good resolution and clean base lines.

# 4

# Experimental Data

This chapter presents the procedures, tools, and techniques for processing the experimental data. Sections will discuss documentation, data processing tracking systems, and how data are actually processed.

## Experimental Results Documentation

Documentation of experimental conditions and results is performed at every level of processing to assure that no data or other useful information is lost and that all data can be processed. Methods have been developed to allow for redundant documentation and to provide the smog chamber operators several different opportunities to document the experiment.

### Data

Data are documented several ways reflecting the different types of data acquisition techniques. Data is acquired and recorded by both computer and stripchart. Printouts are also produced by the computer during and after an experiment and provide additional documentation.

#### *Stripcharts*

Almost every source of data is recorded on stripchart, providing a backup for the computer DA system in case of failure. For instruments that produce data not suitable for the computer DA system, stripchart recorders are the main data acquisition device. All stripcharts are documented with rundate, instrument, time, side, attenuation, chart speed, full scale deflection, and calibration information. Documentation of stripcharts is requested by the setup checklist and performed by the setup operator. Changes of instrument settings or conditions are noted directly on the stripchart during the experiment. Time and side is recorded several times throughout the experiment, as requested by all of the checklists discussed above. A pack-up inventory checklist assures that all stripcharts are collected and stored in the runfolder. Stripchart data is obtained for the following instruments:

- $O_3$ monitor
- $NO_x$ monitor
- Carle 1 GC-FID for HC
- Carle 2 GC-FID for HC
- Carle 3 GC-FID for HC
- Formaldehyde monitor
- Dewpoint monitor
- Varian GC (PAN, tracers, nitrates, biacetyl)
- PE900 GC
- TSR (total solar radiation)/UV sensors

*Printouts*

Printouts produced during and after an experiment also document the experimental data. These are retained in each runfolder:

- `PRINT PROFILE`—computer data dump during run
- Experiment `COMMAND FILE` listing—list of scheduled injections and chamber control commands
- Experiment `BAKTRN FILE` listing—list of actual injections and chamber control commands (both scheduled and manually activated)
- Operator's `REMARKS FILE`- comment file

*Computer Data*

There are two types of computer data generated by this data processing system: computer acquired data during the experiment and files produced from stripchart recorded data after the experiment in data processing. Documentation for computer data exists within the data files produced themselves. Time, instrument, side, and any intermediate conversion factors used to store the data is recorded automatically. The remarks file contains comments entered by the site operators before, during, and after the experiment directly into the computer, which are automatically documented with time entered. The data files produced from stripchart data after the experiment contain all of the documentation recorded on the stripcharts and the name of the people involved in processing the data.

## Forms

Several paper forms are used to help document the experimental conditions and resulting data. Several of these are filled out at the smog chamber site as the experiment is set up and executed.

### *Run Form*

The run form is a major documenting tool. It is used to record all the information needed to determine what experiment was attempted, what the chamber conditions were, time the experiment starts and ends, and important notes about the experiment actually conducted. The form is partially filled out before the experiment to officially record the desired target conditions including sources and amounts of chemical species. The morning operator takes instructions from this form to initiate the experiment, and records important comments about chamber conditions, deviations from target conditions, and any problems. This form is shown in Figure 12.

### *Instrument Checklist Form*

The instrument checklist is filled out the morning of the experiment and is attached to the run form. It is used to indicate which instruments are operational and were used, any calibrations performed, and any problems with the instruments themselves. This form is shown in Figure 13.

### *Run Folder Inventory Checksheet Form*

This form is used to inventory the run folders contents when the runfolder is first logged into the data processing system. It is a primary QA step used in conjunction with the instrument checklist form to determine what data exists, including documentation. Login and filling out of this form occurs before anyone is allowed to work with the contents. This form is shown in Figure 14.

### *Data Processing Instruction Form*

The data processing instruction form is used to collect and convey important information about the data collected on stripcharts during an experiment. It is an intermidiate documenting tool used to indicate start and stop times of valid data, calibration data (not to be confused and picked as run data), species to pick and

## RUN SHEET

Run Date ______________ Project _________ Operator Set-up _____________

Operator Morning _________________ Operator Afternoon _________________

Experiment Number ____________ from Table ____________________________

Command File(s) ____________________________ Tank File Date ____________

Run Description and Purpose ___________________________________________

_______________________________________________________________________

_______________________________________________________________________

_______________________________________________________________________

Special Tasks, Modifications __________________________________________

_______________________________________________________________________

### ACTUAL INJECTION CONDITIONS AND ESTIMATED INITIAL CONCENTRATIONS

Dilution Tracers ID    Blue, ul    Red, ul

_________________    _______    ______

_______________ Blue ________ _________ Red _______________

| Species ID | stat dynam | Concen. Concen. | secs,ul,g ul,liter | dynam ml/min | stat dynam | Concen. Concen. | sec,ul,g ul,liter | dynar ml/m: |
|---|---|---|---|---|---|---|---|---|
| NO | | | | | | | | |
| NO2 | | | | | | | | |
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| | | | | | | | | |
| Total_HC_ | | | | | | | | |
| Total_NOx | | | | | | | | |

Drying Performed? Red ____ Delta Time ____ Blue ____ Delta Time ____

Dew Point(sunrise) Red ____F _____mv Time. _____ Blue _____F _____mv Time __

Morning Chamber Condensation Observed ? (Y/N) Red: inside _____ outside __
Blue: inside _____ outside __

Vent Doors Checked (initials): Morning ______ End of run ______
CHARTS LABEL (initials): Morning ______ End of run ______

Special Problems, Concerns, or Comments _______________________________

_______________________________________________________________________

_______________________________________________________________________

_______________________________________________________________________

_______________________________________________________________________

DVM Data Recorded (TIMES) ______ to ______ Experiment starts (TIME) _____
Experimental Conditions established at (TIME) _______

Run rating (circle one): useless borderline fair good great unknc

Figure 12. Runsheet

Instrument Checklist Run Date ____________________

| Instrument | Cal Today (y/n) (type) | Cal TIME(S) | Opera-tional (check) | Not Opera-tional (check) | Not Used (check) | Data Acqui-sition QA (init.) | Note (num) |
|---|---|---|---|---|---|---|---|
| ATC | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Carle I | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Carle II | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Carle III | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| CEA Formaldehyde | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| CO meter | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Dew Point | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| DNPH Aldehydes | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Nitric Acid | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| NOx Bendix | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Ozone Bendix | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| PE 900 (chamber) | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Saltzman | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Temp | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| TSR | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| UV | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Varian aerosol | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Varian gas | | | | | | | |
| PAN | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Nitrates | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Tracer | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Other | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Other | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Other | ____ | ____ | ____ | ____ | ____ | ____ | ____ |
| Other | ____ | ____ | ____ | ____ | ____ | ____ | ____ |

# Notes

__ ________________________________________
__ ________________________________________
__ ________________________________________
__ ________________________________________
__ ________________________________________
__ ________________________________________
__ ________________________________________
__ ________________________________________
__ ________________________________________
__ ________________________________________
__ ________________________________________
__ ________________________________________

**Figure 13.** Instrument Checklist Form

RUN FOLDER INVENTORY CHECKSHEET INIT: ________ RUN DATE: ____________

PROJECT: AUTO DODG REAC WOOD DATA: AERO GAS WOOD

| PRESENT | ITEM | COMMENTS |
|---|---|---|
| | Run sheet | |
| | Instrument Checklist | |
| | ATC stripchart* | |
| | Carle I stripchart* | |
| | Carle II stripchart* | |
| | Carle III stripchart* | |
| | CO meter stripchart* | |
| | Dewpoint stripchart | |
| | FORM stripchart* | |
| | NO stripchart | |
| | NO2 stripchart | |
| | O3 stripchart | |
| | PE900 stripchart* | |
| | PRINT PRO printout | |
| | .R CMANDR printout | |
| | .R DATRAN printout | |
| | .R MERGE printout | |
| | Sigma 10 printout | |
| | TSR stripchart | |
| | UV stripchart | |
| | Varian stripchart* | |
| | DNPH ald stripchart* | |
| | OTHER: ____________ | |
| | OTHER: ____________ | |
| | OTHER: ____________ | |
| | OTHER: ____________ | |

**Figure 14.** Run Folder Inventory Checksheet Form

problems in general with the data. Calibration factors and any calculations or notes are indicated on this form. The information on this form eventually ends up in the final segmented file used for distribution. This form is shown in Figure 15.

### *DVMFIX Data Sheet Form*

This form is similar to the Data Processing Instruction Form used with stripchart data. It is used to record and convey important information required to properly process the data recorded with the DVM computer acquisition system. Calibration factors, periods of valid data, and general documentation are indicated here. The information on this form eventually ends up in the final segmented file used for distribution. This form is shown in Appendix E.

## Plots

Plots are a form of documentation as well as a method of presenting data. They indicate when calibrations were performed, when injections were made, and when the chamber is vented. They often indicate power failures, computer failures, or in general problems, and general quality of data.

### *Raw Data Plots ("P"- and "U"-file Plots)*

These are plots of raw uncorrected and at first unQAed data. "P"-file plots show raw "picked" (digitized data). "U" file plots show the raw DVM data, often including the AUTOCAL calibrations and venting. Both types of plots indicate completeness of data, ratios of conditions, profiles and general reasonableness of data. Discontinuities may indicate problems during picking.

### *Processed Data (G- and C-files QA plots)*

These plots of the final corrected data show immediately any problems or errors which might have occured in processing. Only valid experimental data should have been processed. Concentrations should be close to target conditions. Light, dewpoint, and temperature data should be reasonable in magnitude.

### *Tracer Data Plots (CSTAR)*

Inert tracers are usually injected into each chamber half to monitor dilution during the experiment. Raw data are read and processed by a computer program CSTAR which fits the data to an exponential function with the least-squares method. The slope is the dilution rate which should be used by modelers. This data is processed for every run; chamber leaks can be detected quickly.

DATA PROCESSING INSTRUCTION FORM pg _____ of _____

RUN DATE ___________________ INSTRUMENT ___________________

RUN HCANAL (y/n) ____ ON FILES BETWEEN _________ AND _________

| COMPOUND | SIDE | CAL FAC & ATTN (AND UNITS) | CAL FACTOR CALCULATIONS/DOC | INITIAL/ DATE |
|---|---|---|---|---|
| | | | | |
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| | | | | |

Cal Source Reports Used ______________________________ Date ________________

Cal Source Reports Used ______________________________ Date ________________

Cal Source Reports Used ______________________________ Date ________________

RECORD ANY SPECIAL NOTES OR CALCULATIONS ON BACK OF THIS FORM PLEASE !

Figure 15. Data Processing Instruction Form

## Run Data Processing Status Databases

### *Description of Lab/Site Calenders*

Calendars have been discussed above. They are used as a primary documenting method. Experiments, calibrations, and some instrument or chamber work are indicated on the calendars at the site and the data processing office first. These are used to guide the data processing effort.

### *Description of* RUNENTRY *database*

A DATATRIEVE database maintained on the VAX is used to track all data processing and record the experimental conditions. The processing status of a single experiment or a group of experiments can be quickly assessed. It is used with report procedures to guide processing tasks. Tasks are listed by the priority given by a project coordinator.

The RUNENTRY system is a PL/I program that runs on the VAX-11/780 computer in the SPH. It provides on-line, interactive access to the database of run processing status. The program uses the VAX "electronic" Forms Management System to support a number of "forms" on a video display unit (terminal). The user can fill out the form, and the data are either called up from the database, or are stored in the database for future reference.

Table 14 is the individual record description for an entry in the database. In addition to the general information about the run conditions, the status of the processing steps for digital voltmeter data, for documentation preparation, for the processing of each instrument that had valid data, and for the progress toward creating the final file are stored in a record for each run.

There are a possible total of 110 checkpoint steps in processing a run. The events that are entered will be listed in sections following. The record provides for nine instruments, accounting for most of the checkpoints.

Single page printouts (132 columns wide) can be created for each run. An example of a printout is shown in Table 15. This shows a nearly completely processed run that had five instruments.

Figure 16, Figure 17, Figure 18, and Figure 19 are "hardcopies" of the terminal screen showing the "electronic" forms. These are designed to be used on terminal that have video attributes such as reverse fields (shown in the figures as dark areas), bold letters (not shown in figures), blinking areas and letters for attention. Each form also has on-line HELP for each field, and if more help is needed, the screens have full-screen help forms with such information as legal key values and HC species numbers.

Several report procedures have been developed to help guide the data processing. These look up the status in `RUNENTRY` for specific tasks for each "type" of personnel: `PCREPORTS`, `PPREPORTS`, `CTREPORTS`. These were explained in Chapter 2. An example of the `PCREPORT` is shown in Figure 20.

Table 14. Record Description for RUNENTRY Database System.

```
01 RUN_REC.
 02 GENERAL.
   03 RUN_DATE        USAGE IS DATE
      EDIT_STRING IS DD-MMM-YYYY.
   03 CONDITIONS      OCCURS 2 TIMES.
      06 SIDE         PIC X(4).
      06 NOXCONC      PIC 9.999.
      06 HC           OCCURS 3 TIMES.
         09 HCCONC      PIC 99.99
            MISSING VALUE IS 0.00
            EDIT_STRING IS  Z9.00?"      ".
         09 SPECIES   PIC 999.
   03 PROJECT         PIC X(4).
   03 QUALITY         PIC 9.
   03 PRIORITY        PIC 9.
 02 DETAIL.
   03 DVMDATA.
      06 ITEM         OCCURS 10 TIMES.
         09 DVEVENT     PIC X(3)
            DEFAULT IS "non"
            VALID IF DVEVENT IN DVEVENT_TAB.
         09 DVEDATE     USAGE IS DATE
            EDIT_STRING IS DD-MMM-YY.
         09 DVINIT      PIC X(3).
   03 DOCUMENTATION.
      06 ITEM         OCCURS 5 TIMES.
         09 DOEVENT     PIC X(3)
            DEFAULT IS "non"
            VALID IF DOEVENT IN DOEVENT_TAB.
         09 DOEDATE     USAGE IS DATE
            EDIT_STRING IS DD-MMM-YY.
         09 DOINIT      PIC X(3).
   03 FINAL_FILE.
      06 ITEM         OCCURS 5 TIMES.
         09 FFEVENT     PIC X(3)
            DEFAULT IS "non"
            VALID IF FFEVENT IN FFEVENT_TAB.
         09 FFDATE     USAGE IS DATE
            EDIT_STRING  IS DD-MMM-YY.
         09 FFINIT      PIC X(3).
   03 PICKDATA.
      06 TOTAL_SPECIES   PIC 99.
      06 NUM          PIC 9
         MISSING VALUE IS 0.
      06 INST         OCCURS 0 TO 9 TIMES DEPENDING ON NUM.
         09 ID        PIC X(3).
         09 ITEM      OCCURS 10 TIMES.
            11 PIEVENT PIC X(3)
               DEFAULT IS "non"
               VALID IF PIEVENT IN PIEVENT_TAB.
            11 PIDATE USAGE IS DATE
               EDIT_STRING IS DD-MMM-YY.
            11 PIINIT  PIC X(3).
```

## Table 15.

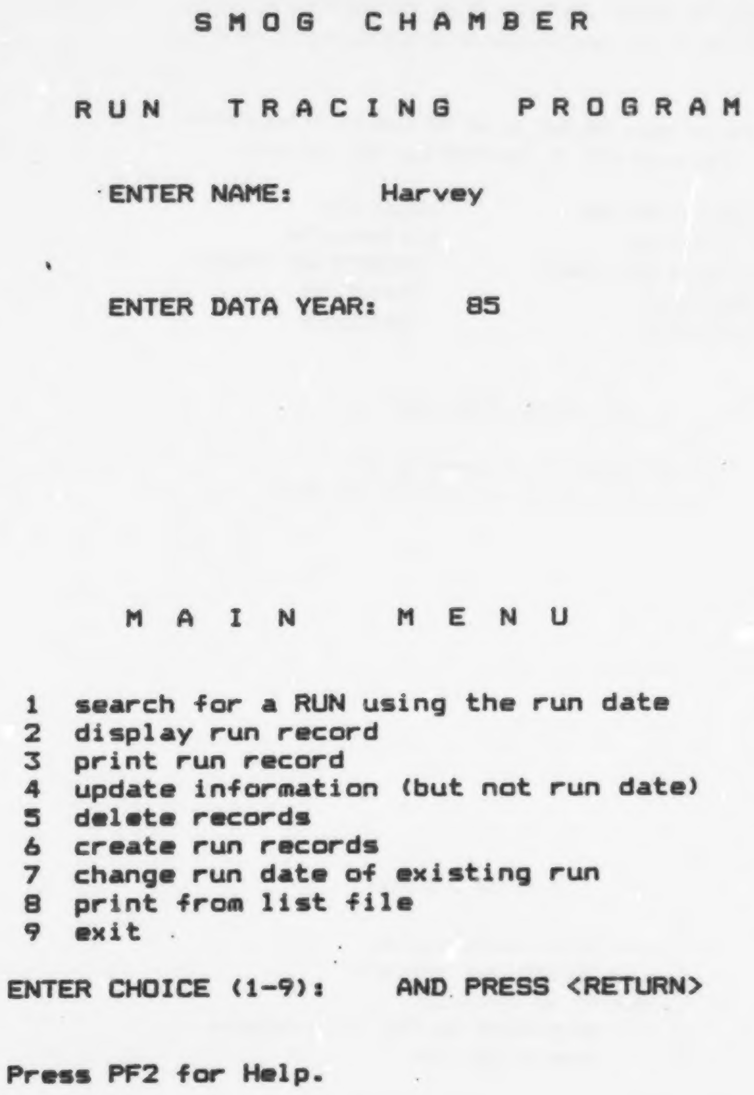
## RUNENTRY Processing Summary for September 14, 1981

```
                         Run Date: 14-SEP-1981    Project: REAC     Quality: 0     Priority: 9
SIDE   NOX      HCCONC   SPECIE  NAME                                SIDE   NOX      HCCONC   SPECIE  NAME
RED    0.300      2.60    191    Uncmix                              BLUE   0.300      2.72    191    Uncmix
                 00.71    068    M-xylene                                             00.71    070    1,2,4-trimethylbenzene
                 00.00    000                                                         00.00    000

--------COMPLETED DVM EVENTS---------    ---------COMPLETED DOC EVENTS---------     ----COMPLETED FINAL FILE EVENTS-----
URV Unpack pgm run  12-OCT-1981 MOS      SUM Run Sumry compl 29-OCT-1982 KGS        MR3 3 sects merged   9-JAN-1983 HEJ
V2T AL tape created             MOS      D2V Doc tran to VAX  7-JAN-1983 KGS        U2T ML tape created 10-JAN-1983 HEJ
RPC Raw Plot creatd             RFP      V2T AL tape created  9-JAN-1983 RFP
POA Plot QA compltd             KGS      T2D Tape trn to dsk  9-JAN-1983 HEJ
CFS Cal facs determ 29-DEC-1981 KGS      DOA Doc QA completd  9-JAN-1983 HEJ
DRU DVMFIX pgm run   7-JAN-1983 RFP
COA Conc QA compltd  7-JAN-1983 KGS
R2M Ready to merge   9-JAN-1983 HEJ

----COMPLETED INSTRUMENT EVENTS-----     ----COMPLETED INSTRUMENT EVENTS-----       ----COMPLETED INSTRUMENT EVENTS-----
Instrument:  C1G Carlo I GC              Instrument:  C2G Carlo II GC               Instrument:  FOG CEA Formaldehyde
PID Pick instrc det 18-MAY-1982 KGS      PID Pick instrc det 18-MAY-1982 KGS        PID Pick instrc det 18-MAY-1982 KGS
PRU PICK pgm run    27-OCT-1982 JLH      PRU PICK pgm run     5-APR-1982 JLH        PRU PICK pgm run     7-APR-1982 JLH
FPT Fast plot creat 27-OCT-1982 JLH      FPT Fast plot creat  5-APR-1982 JLH        FPT Fast plot creat  7-APR-1982 JLH
POA Fst plt QA comp 28-OCT-1982 KGS      POA Fst plt QA comp 28-OCT-1982 KGS        POA Fst plt QA comp             KGS
CFD Cal facs determ 25-MAY-1982 KGS      CFD Cal facs determ 25-MAY-1982 KGS        CFD Cal facs determ  1-JUL-1982 KGS
CRU CALCON pgm run  27-OCT-1982 JLH      CRU CALCON pgm run   8-SEP-1982 CDH        CRU CALCON pgm run   8-SEP-1982 KGS
HRU HCANAL pgm run  27-OCT-1982 JLH      HRU HCANAL pgm run   8-SEP-1982 CDH        COA Comp Chksht QA  28-OCT-1982 KGS
COA Comp Chksht QA  27-OCT-1982 KGS      COA Comp Chksht QA  28-OCT-1982 KGS        F2V Files tr to VAX  7-JAN-1983 RFP
F2V Files tr to VAX  7-JAN-1983 RFP      F2V Files tr to VAX  7-JAN-1983 RFP        V2U Ready to merge   9-JAN-1983 HEJ
V2U Ready to merge   9-JAN-1983 HEJ      V2U Ready to merge   9-JAN-1983 HEJ

----COMPLETED INSTRUMENT EVENTS-----     ----COMPLETED INSTRUMENT EVENTS-----       ----COMPLETED INSTRUMENT EVENTS-----
Instrument:  V2G Varian GC (gas)         Instrument:  COG Beckman 6000 (CO)
PID Pick instrc det 18-MAY-1982 KGS      BAD Stop processing 18-MAY-1982 KGS
PRU PICK pgm run     7-APR-1982 JLH
FPT Fast plot creat  7-APR-1982 JLH
POA Fst plt QA comp             KGS
CFD Cal facs determ 21-MAY-1982 KGS
CRU CALCON pgm run  15-OCT-1982 JLK
COA Comp Chksht QA  28-OCT-1982 KGS
F2V Files tr to VAX  7-JAN-1983 RFP
V2U Ready to merge   9-JAN-1983 HEJ
```



```
          S M O G   C H A M B E R

      R U N   T R A C I N G   P R O G R A M

       ENTER NAME:     Harvey


       ENTER DATA YEAR:     85





         M A I N   M E N U

   1  search for a RUN using the run date
   2  display run record
   3  print run record
   4  update information (but not run date)
   5  delete records
   6  create run records
   7  change run date of existing run
   8  print from list file
   9  exit

  ENTER CHOICE (1-9):    AND PRESS <RETURN>

  Press PF2 for Help.
```

Figure 16. Runentry Welcome and Main Menu Screens

```
                 S E L E C T   A   R U N

         ENTER THE DESIRED RUN DATE: 05-aug-1984 AND PRESS <RETURN>.
          (A run did not have to occur on this date, but it helps.)


        If the following Run_Date is not the same as the one entered,
            then a run with the requested date does not exist.

        Run_Date  5-AUG-1984            Project METH
        Red Hydrocarbon                 Blue Hydrocarbon
          SYNTHETIC AUTO EXHAUST          SYNTHETIC AUTO EXHAUST
          AROMATIC MIX                    AROMATIC MIX
          FORMALDEHYDE                    FORMALDEHYDE


                 IS THIS THE CORRECT RUN ?  y

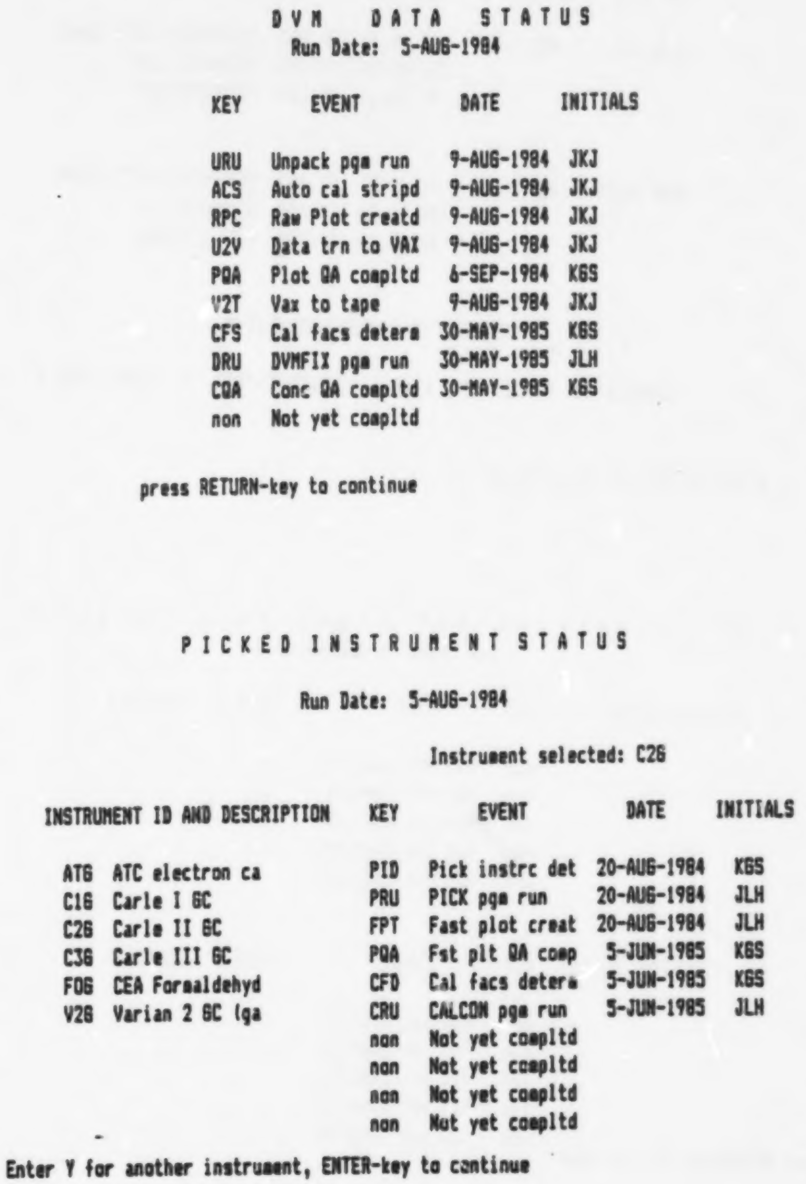
            (Y) yes, establish as current run_date
            (L) no, leave search and return to main menu
```

```
                      SELECTION OF DISPLAY

             1  show GENERAL run information
             2  show INSTRUMENT run information
             3  show DVM run information
             4  show DOCUMENTATION and FINAL FILE information
             5       return to main menu

         ENTER CHOICE (1,2,3,4, or 5):    AND HIT <RETURN>
```

**Figure 17.** RUNENTRY Date and Display Selection Screens



```
                    D V M   D A T A   S T A T U S
                      Run Date:  5-AUG-1984

                  KEY      EVENT          DATE      INITIALS

                  URU  Unpack pgm run    9-AUG-1984  JKJ
                  ACS  Auto cal stripd   9-AUG-1984  JKJ
                  RPC  Raw Plot creatd   9-AUG-1984  JKJ
                  U2V  Data trn to VAX   9-AUG-1984  JKJ
                  PQA  Plot QA compltd   6-SEP-1984  KGS
                  V2T  Vax to tape       9-AUG-1984  JKJ
                  CFS  Cal facs determ  30-MAY-1985  KGS
                  DRU  DVMFIX pgm run   30-MAY-1985  JLH
                  CQA  Conc QA compltd  30-MAY-1985  KGS
                  non  Not yet compltd

          press RETURN-key to continue
```

```
               P I C K E D  I N S T R U M E N T  S T A T U S

                           Run Date:  5-AUG-1984

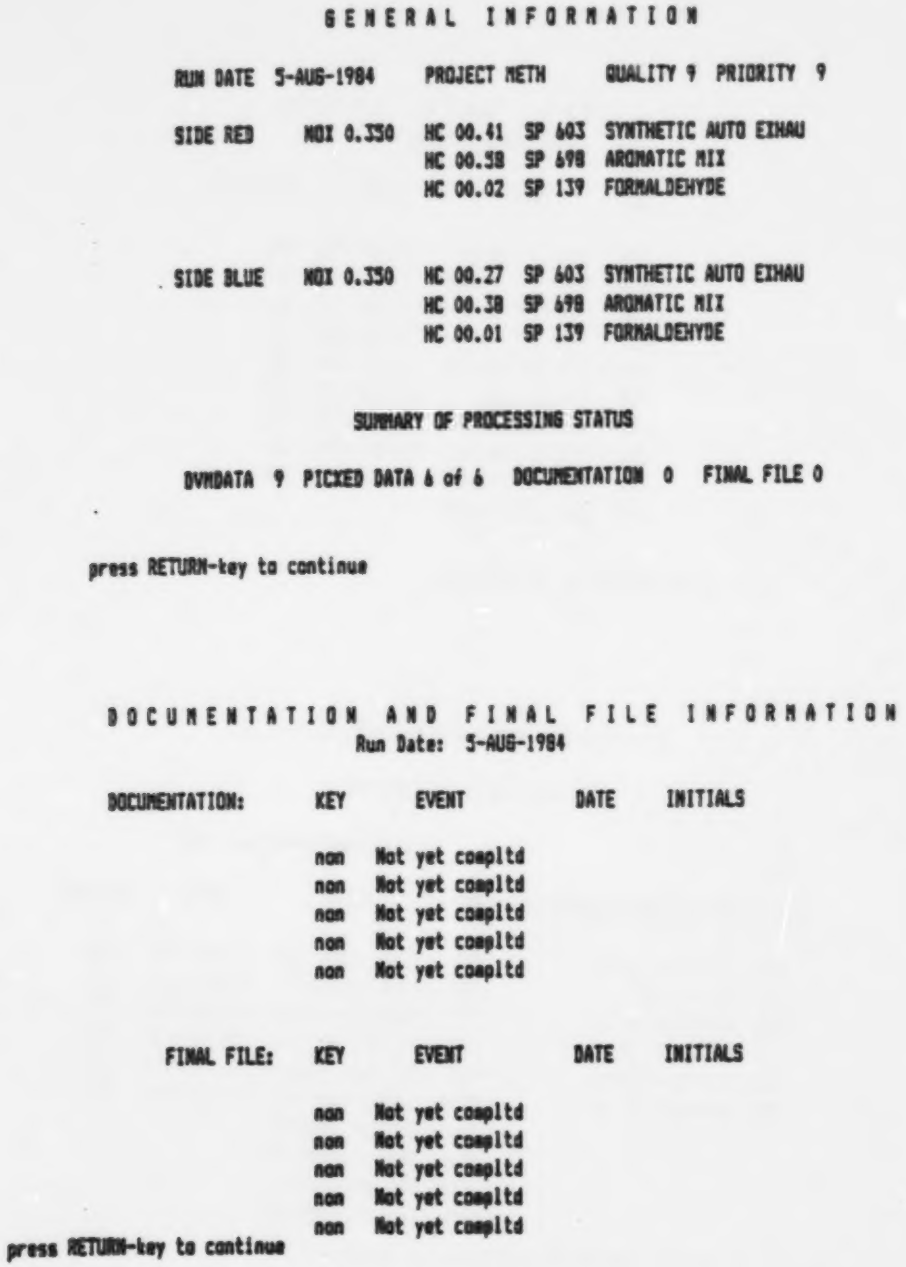
                                         Instrument selected: C2G

    INSTRUMENT ID AND DESCRIPTION   KEY      EVENT          DATE      INITIALS

     ATG  ATC electron ca           PID  Pick instrc det  20-AUG-1984   KGS
     C1G  Carle I GC                PRU  PICK pgm run     20-AUG-1984   JLH
     C2G  Carle II GC               FPT  Fast plot creat  20-AUG-1984   JLH
     C3G  Carle III GC              PQA  Fst plt QA comp   5-JUN-1985   KGS
     FOG  CEA Formaldehyd           CFD  Cal facs determ   5-JUN-1985   KGS
     V2G  Varian 2 GC (ga           CRU  CALCON pgm run    5-JUN-1985   JLH
                                    non  Not yet compltd
                                    non  Not yet compltd
                                    non  Not yet compltd
                                    non  Not yet compltd

 Enter Y for another instrument, ENTER-key to continue
```

**Figure 18.** RUNENTRY General, Documentation, and File Status Screens



```
                    G E N E R A L   I N F O R M A T I O N

        RUN DATE  5-AUG-1984     PROJECT METH       QUALITY 9  PRIORITY  9

        SIDE RED      NOX 0.350   HC 00.41  SP 603  SYNTHETIC AUTO EXHAU
                                  HC 00.58  SP 698  AROMATIC MIX
                                  HC 00.02  SP 139  FORMALDEHYDE


        SIDE BLUE     NOX 0.350   HC 00.27  SP 603  SYNTHETIC AUTO EXHAU
                                  HC 00.38  SP 698  AROMATIC MIX
                                  HC 00.01  SP 139  FORMALDEHYDE

                         SUMMARY OF PROCESSING STATUS

         DVMDATA  9  PICKED DATA 6 of 6   DOCUMENTATION  0   FINAL FILE 0


  press RETURN-key to continue
```

```
      D O C U M E N T A T I O N   A N D   F I N A L   F I L E   I N F O R M A T I O N
                              Run Date:  5-AUG-1984

      DOCUMENTATION:       KEY       EVENT            DATE     INITIALS

                           non   Not yet compltd
                           non   Not yet compltd
                           non   Not yet compltd
                           non   Not yet compltd
                           non   Not yet compltd

              FINAL FILE:  KEY       EVENT            DATE     INITIALS

                           non   Not yet compltd
                           non   Not yet compltd
                           non   Not yet compltd
                           non   Not yet compltd
                           non   Not yet compltd
press RETURN-key to continue
```

**Figure 19.** RUNENTRY DVM and Picked Instrument Status Screens

**Figure 20. PCreport Example**

```
Count of runs that have reached stated stages of processing
          for ALLRUN84
Total runs Total Inst
   63        312
******** DVN data ************
URU RPC ACS NAC U2V V2T PQA CFS DRU CQA R2M NTB BAD NDV
 58  58  58   0  57  57  54  38  37  37   0   2   1   3
     Sum of URU, NTB, and NDV is   63
######## Inst data ############
PID PRU FPT PQA CFD CRU HRU CQA F2V V2U NTB BAD
190 190 190 116 104 104   0  17   0   0 135   6
     Sum of PID and NTB is  325
######## Documentation ############
SUM D2V DQA
  7   7   2
######## Final File ############
MR3 ALT FQA
  0   0   0
Number of P-files should be : 190
Number of C-files should be : 104
Number of K-files should be : 104
```

### Figure 20(cont.). PCreport Example

```
ALLR runs/instuments needing Picking Instructions Determined (PID).
      This is an INST first processing stage report.
------------------------------------------------------------
                           PRIORITY >>> 8 <<<
         26-Jun-84  Number of inst =   8
              PCG  PE 900 GC
                   (chamber)
------------------------------------------------------------
                           PRIORITY >>> 5 <<<
         25-Jun-84  Number of inst =   8
              PCG  PE 900 GC
                   (chamber)
     ALLR runs/instuments needing Cal Factors Determined (CFD).
    The following instruments have ( PID ) Pick inst det completed
                            but not ( CFD ) Cal fac det completed.
            RUN
            DATE        Instruments             Date done     Person
------------------------------------------------------------
                           PRIORITY >>> 9 <<<
         25-Jul-84  Number of inst =   5
              V2G  Varian GC (gas)
                    PID    Pick inst det         6-Aug-84      KGS
------------------------------------------------------------
                           PRIORITY >>> 5 <<<
         25-Jun-84  Number of inst =   8
              COG  Beckman 6800 (CO)
                    PID    Pick inst det        31-Jul-84      JA
              V2G  Varian GC (gas)
                    PID    Pick inst det        31-Jul-84      JA
```

## Description of Data Processing Status Database

This section describes the data processing status database and how it is used.

### Description

The main parts of the data processing status database are the calendars and the RUNENTRY DATATRIEVE system. RUNENTRY maintains status information for each experiment by date. The general categories are:

- GENERAL
    - experimental chemical conditions for both sides,
    - quality and priority index,
    - number of experiments
- INSTRUMENT
    - pick instructions,
    - cal factors given,
    - qa performed,
    - final processing steps performed;
- DVM
    - unpacking performed,
    - cal factors given,
    - QA steps performed,
    - final processing performed;
- DOCUMENTATION
    - final documentation processed and written,
    - moved to VAX for final segfile formation.

### Use of Data Processing Status Database

This section describes how the database is used from the time the experiment is conducted to final processing.

#### *Log Experiment*

When an experiment is conducted (attempted), the conditions and general quality are indicated on both calendars (site and office). This information is usually obtained by telephone conversations between the project coordinators and site personnel within a few hours after the start of the experiment in order to plan for the next days activities. Another late afternoon telephone conversation follows to determine the outcome of the experiment and to finalize the next days plans. If the experiment is thought to be successful or might provide any the useful information, it is considered to exist. The absence of major negative comments such as "failure" written on the calendar, triggers the data processing procedure. The experiment is packed-up and inventoried if it is not considered a "failure" for transport to the dataprocessing office.

From the telephone conversation mentioned above, the experiments success is determined. If the experiment is considered worth archiving, the actual experiment conditions and general quality are recorded on the calendars. Otherwise the attempted experiment and the problems associated are noted on the calendar.

Data processing personel expect both the runfolder and data floppies to be transported to the school within a few days after the experiment. Special locations in the office are set aside for incoming data. The calendars and these areas are checked daily. If data is late, the site personel are contacted and questioned. When either the run folder or data floppies arrive at the office, the experiment is entered into the RUNENTRY database.

The contents of the runfolder are first inventoried before any data processing occurs. The instrument checklist completed during the experiment is compared with the folder contents. Missing items are investigated.

### *Preliminary Review*

Preliminary review usually begins the day or day after an experiment is conducted by a PC. Conversations with the site operators indicate resulting experimental conditions and outcome and any problems which might have occured. The run folder contents are inspected. Instrument operation behavior, chamber background(proper venting, drying or absence of condensation), temperature and dewpoint, sunlight, initial conditions, and reasonableness of results are determined. Basic quality and processing priority is determined. Completeness for data and documentation is determined. The calendars and the RUNENTRY database are updated. Besides a QA step for the experiment itself, the success of meeting the experimental plan goals is checked. A variation in the experiment might be useful if documented but would result in rescheduling of the target experiment.

### *Processing Instructions and Information*

RUNENTRY is used to track data processing by recording of processing events. Automatic status reports can be generated. Report procedures are used to guide and assign processing tasks: PCREPORTS, PPREPORTS, and CTREPORTS. The reports are listed by priority (0-9) as determined by the PC.

PCREPORTS tells the project coordinators that picking instructions are needed, or picked data exists and needs QA and calibration factors, or final data exists and needs QA. CTREPORTS indicates to the computer technicians that DVM data needs unpacking and archival, and AUTOCAL data needs to be stripped. PPREPORTS tells the peakpickers that pick instructions have been given, or that picked data has been QAed and calibration factors exist for final processing.

Each worker updates RUNENTRY as each step is performed. The presence of each new step completed generates instructions to the next appropriate worker to perform the next processing task when a new report is generated. When all processing steps are completed, the segmented file is assembled, and the final initial experimental conditions and quality are updated in the RUNENTRY GENERAL section. This data is input to the RUNSUMMARY database which is used to sort, organize, and analyze the total smog chamber experimental database.

## Digital Voltmeter Data Processing

The Digital Voltmeter Data (DVM) from the Computer DA system is usually processed easily once the calibration database is established. The processing flowchart is indicated in Figure 21. The RUNENTRY events flowchart is shown in Table 16.

The computer technician (CT) "unpacks" the data from the two floppies which arrive from the research site. Several files generated by the site DA system are copied to the LSI-11 harddisk: the main DVM file (mmddy.DVM), the remarks file (mmddy.REM), the command file (mmddy.CMD), the adjustments file (mmddy.ADJ), and the file of actual computer commands (mmddy.OPS). Printouts of all of these files except the mmddy.DVM file are made and stored in the RUNFOLDER. A computer program (UNPACK) is run which produces a "U" file, which is the same raw data but in ASCII format and is the principle raw data file for the smog chamber experiment. This file contains 24 hours of data taken every minute for every instrument connected to the DVM. The "U" file is back-up onto two sets of floppies, and to two types of magnetic tape used on different computers: the VAX-780 and the University's IBM 4381.

Several programs are used to process data from the "U-file". FASTDV is run several times: to produce "P" files for plotting the raw data ("fastplots") from the experiment and to strip the AUTOCAL data (makes "A" file). The processing of the calibration data was discussed earlier. PLOPIC is used to make the plots from the "P" files for the $NO_x/O_3$ plot and the TSR/UV, temperature, and dewpoint plot. Theses plots are stored both in the RUNFOLDER and the FASTDV notebook. All of the

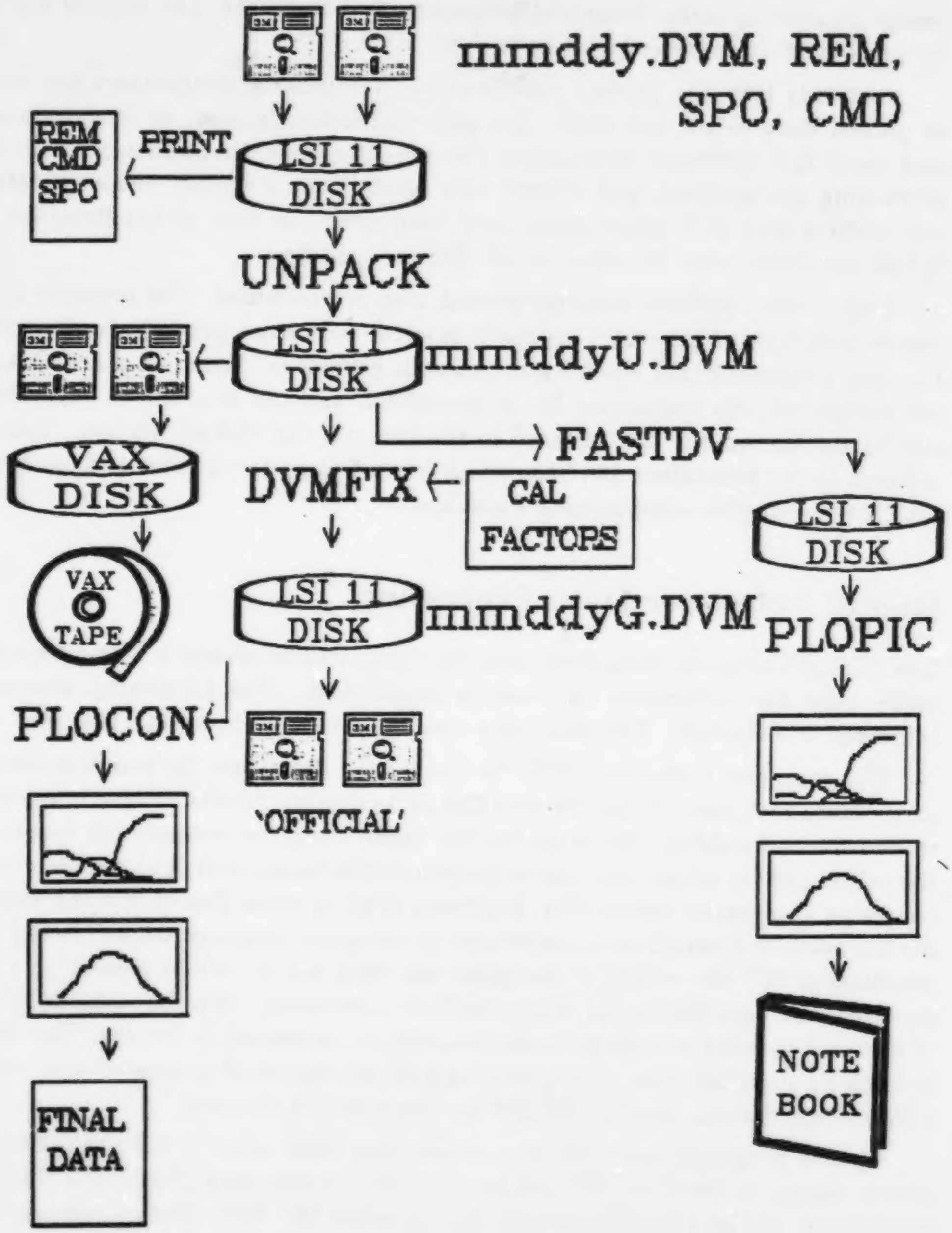

mmddy.DVM, REM,
SPO, CMD
REM
CMD
SPO
PRINT
LSI 11
DISK
UNPACK
LSI 11
DISK
mmddyU.DVM
FASTDV
VAX
DISK
DVMFIX
CAL
FACTORS
LSI 11
DISK
VAX
TAPE
LSI 11
DISK
mmddyG.DVM
PLOPIC
PLOCON
'OFFICIAL'
NOTE
BOOK
FINAL
DATA

**Figure 21.** DVM Processing Flowchart (Computers and Files)

## Table 16.

## Processing System for DVM Data

```
 cal processing
 /             \
tot runs       (CFS)-------
 \             /            \
  \       (ACS)              \
   \     /                    \
   (URU)------(RPC)----!PQA!-<DRU>--!CQA!--!R2N!
        \                     /
         (UTV)               /
              \             /
               (V2T)-------
```

```
!sss! == stages determined by Project coordinator (PC)
<sss> == stages determined by Peak Pickers (PP)
(sss) == stages determined by Computer Techs (CT)
```

DVM data processing steps

| Pers | Step | Meaning |
|---|---|---|
| CT | URU : Unpack run | Site floppy data expanded to ASCII Ufiles |
| CT | U2V : Data to VAX | Ufiles moved from LSI disk to VAX |
| CT | V2T : to archive tape | Data moved from VAX to tape |
| CT | RPC : Raw Plot done | Plot of voltages to examine data |
| PC | PQA : Plot QA | Initial quality check |
| CT | ACS : AutoCals strip | Cals separated for processing |
| PC | CFS : Cals done | Calibration factors determined |
| CT | DRU : DVMFIX run | Voltages changed to concentrations |
| PC | CQA : Conc QA | Concentration Quality Assurance |
| CT | R2M : Ready 2 merge | Merge process on VAX can be run |
| PC | NTB : Not to be proc | Not to be processed |
| PC | BAD : Stop processing | Something is wrong with this data |
| CT | NDV : No DVM data | |

tasks discussed so far are done by the CT. The CT update RUNENTRY as these tasks are performed.

When the FASTDV plots are made and RUNENTRY has been updated so, the PCREPORT will direct the PC to perform a QA on the raw data. The plot is compared with the original stripcharts. If data is missing, the documentation (RUNSHEETS, REMARKS FILES, INSTRUMENT CHECKLIST, CALENDARS) is investigated for mention of power or computer failures, or instrument malfunction. The data may need to be retransfered from the site. Missing data may have to digitized from the stripcharts. Once the raw data is QAed, the PC updates RUNENTRY that the raw data has been unpacked successfully (PQA) and calibration factors can be applied (calibration factors need to be determined).

Calibration factors are applied to raw DVM data with a program called DVMFIX which runs on the LSI computer. The program also controls which time periods of raw data are processed. Bad data, or cal data is eliminated in this way. Calibration factors are obtained from a list resulting from calibration factor processing discussed above. Interpolation may be required. Usually however $NO_x$ and $O_3$ monitors are calibrated twice a day, before and after each experiment. The calibration factors can be used directly.

The PC fills out a DVMFIX sheet indicating the calibration factors to apply to the data, the periods of valid data to process, and brief documentation. The calibration factors are obtained from the AUTOCAL report as described above. The PC updates RUNENTRY that calibration factors have been determined. The information on the DVMFIX sheet is transfered to a file on the LSI-11 computer (mmddy.CRD) usually by a PP or CT. The "U" file is moved back to the harddisk. This might require the assistance of the CT if these files are not still on floppies and need to be copied off of one of the magnetic tapes. The program DVMFIX is used to apply the calibration data in the mmddy.CRD file to the raw data, producing a new file of corrected data for only valid experimental data for every fourth minute (mmddyG.DVM "G-file"). DVMFIX is usally run by the person who creates the mmddy.CRD file. The "G-files" are backed-up on floppies. RUNENTRY is updated that DVMFIX has been run and final QA is need by the PC.

The final corrected data is listed and plotted. Concentration data for NO and $NO_2$ must equal $NO_x$ concentrations within a few ppb throughout the experiment. "Zeros" are checked. Initial conditions are compared with the target conditions. Dewpoint, and temperature data are checked for consistency and reasonableness (dewpoint data cannot be higher than chamber temperature). Profiles and maximum values of light are compared with other seasons for resonableness. Data not to be processed or missing should have "-9.9999" indicated. If there are problems, the PC will re-issue processing instructions, deleting from RUNENTRY that DVMFIX has been run. This will cause the PPREPORTS and CTREPORTS to request that the data be reprocessed. The process is repeated until the QA criteria are satisfied.

## Strip Chart Data Processing

Processing strip chart data is a little more complex than processing DVM data. More data is represented, more calibration factors are required, and there are more sources of error. Basically the data are identified, the conditions of the instruments are identified, the data is picked (digitized), plotted, and QAed, calibration factors are determined and applied, and the final data is listed and plotted for final QA. The processing flowchart is indicated in Figure 22. The RUNENTRY events flowchart is shown in Table 17.

Data processing starts with RUNENTRY indicating to the PC in the PCREPORT that pick instructions are needed for the instruments used in an experiment. Data processing starts with the documentation. The RUNSHEET and RUNENTRY indicate which species where injected for the experiment. The instruments which require processing are identified. The stripcharts are investigated for proper documentation: attenuation, chart full scale setting and chart speed, time, and chamber side sampled. The chromatograms are inspected for proper appearance (operation). The background chromatograms are inspected for contamination. Major problems are noted. If the data is valid but not useful the NTB is indicated in RUNENTRY. If the data is bad, BAD is indicated. No further action will be taken.

If the instrument seems to be free of problems and data are considered useful, then pick instructions are given. Calibration data are identified and noted as not to be processed by the peakpicker (PP). The compounds monitored and their peaks are identified and labeled. The entire stripchart is inspected for reasonable appearance and operation and data. Problems are identified and noted. The peakpicker can indicate in the data that data are missing (off-scale, power failure, instrument adjustment, *etc.*). The start and end times of valid data are identified. The compounds to be picked are listed on the DATA PROCESSING INSTRUCTION FORM with any additional instructions. RUNENTRY is updated with PID (pick instructions determined) by the PC. This indicates in the PPCREPORT to the PP that data is ready to be picked.

The PP obtains the run folder and determines from the DATA PROCESSING INSTRUCTION FORM which compounds are to be picked. The stripchart is removed and spread out over the digitizer pad. Using the instructions and peak identification on the stripchart the data is digitized using the program DIGPIK run on the LSI-11 computer to produce a file named mmddyP.iit ("P" file). The files are backed-up on floppies and magnetic tape. The data is then plotted with a program called PLOPIC on the LSI-11 with GIGI graphics. A hardcopy is stored in the RUNFOLDER. The PP updates

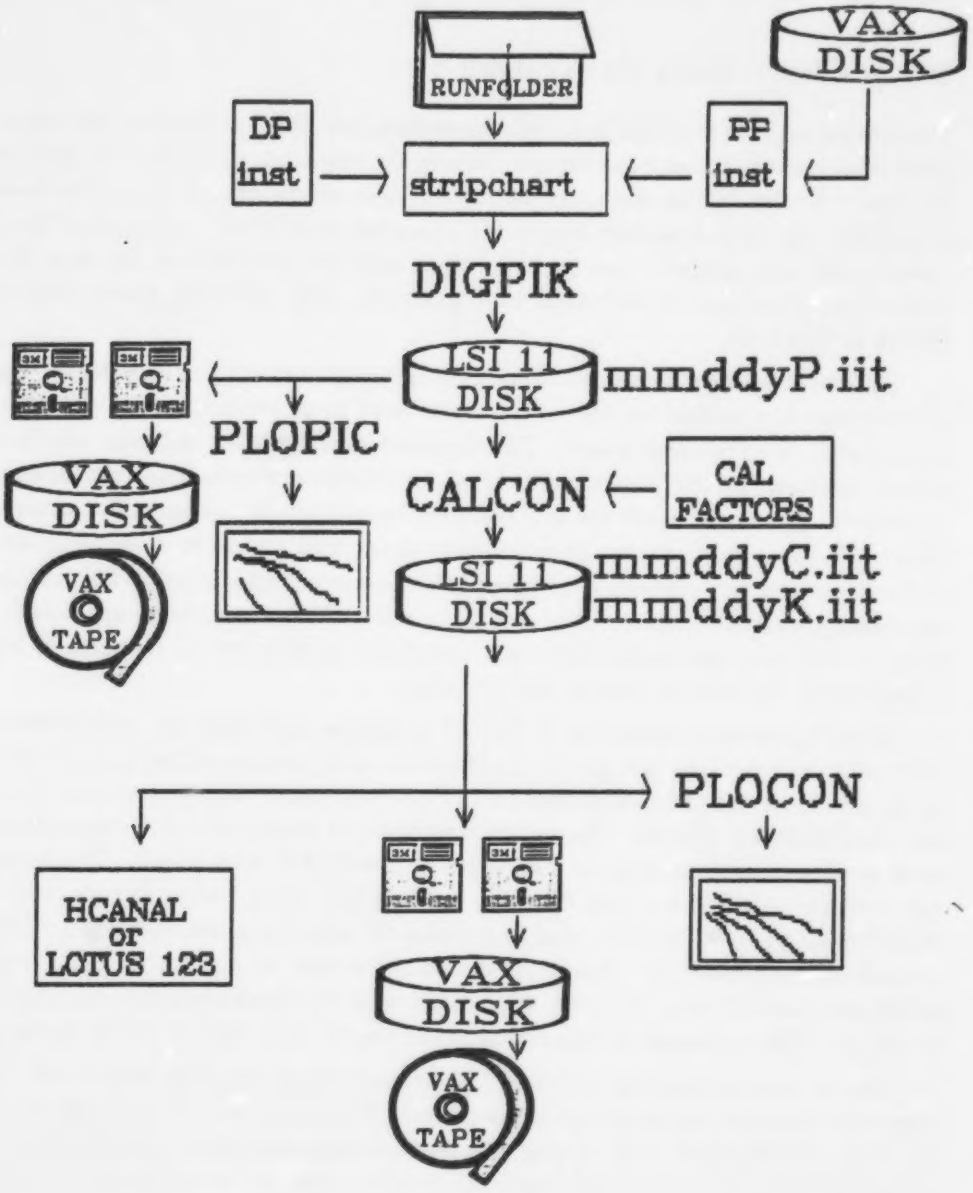

RUNFOLDER
VAX DISK
DP inst
stripchart
PF inst
DIGPIK
LSI 11 DISK
mmddyP.iit
PLOPIC
VAX DISK
VAX TAPE
CALCON
CAL FACTORS
LSI 11 DISK
mmddyC.iit
mmddyK.iit
PLOCON
HCANAL or LOTUS 123
VAX DISK
VAX TAPE

**Figure 22.** Instrument Processing Flowchart (Computers and Files)

## Table 17.
## Processing System for Instrument Data

```
      !NTB!
     /
   tot inst  __ cal processing_
     \     /                  \
      !PID!                   !CFD!      <HRU>__
        \                         \     /       \
         \                         <CRU> -------- !CQA!---- (F2V)---- (V2U)
          \                        /
           <PRU>---- <FPT> --!PQA!
```

```
!sss! == stages determined by Project coordinator (PC)
<sss> == stages determined by Peak Pickers (PP)
(sss) == stages determined by Computer Techs (CT)
```

| Pers | RUNENTRY stages | Meaning |
|---|---|---|
| PC | PID : Pick inst det | Charts marked, Inst status sheet in folder |
| PC | NTB : Not to be proc | No futher processing marked on Inst Status sheet |
| PC | CFD : Cal fac det | Cal factors for each comp entered on Inst status sheet in folder |
| PP | PRU : Pick run | Data has been digitized and P-file exists |
| PP | FPT : FPlot done | P-file has been plotted and plot is in folder |
| PC | PQA : FPlot QA | Fast plot has been marked OK (no bad data points in P-file) |
| PP | CRU : CALCON run | C and K files exist on floppies |
| PP | HRU : HCANAL run | HC analysis printout in run folder |
| PC | CQA : Comp CS QA | Instrument QA completed on C and K files<br>Initial Conditions updated |
| CT | F2V : File 2 VAX | C and K files moved to VAX |
| CT | V2U : Ready 2 merge | C files merged together, K files merged together |
| PC | BAD : Stop processing | Something is wrong with this data |

RUNENTRY that the data has been picked (PRU: pick run) and a "fastplot" has been made (FPT). This indicates in the PCREPORT to the PC that raw data has been picked and requires QA.

The "fastplot" is inspected and compared with the original stripchart. Appropriate chemical behavior is noted. The stripchart data is compared to assure that the data is picked correctly: time and side for chromatograms and amplitude of peaks. When possible, picked data is inspected for consistency: similar compounds on the different sides should show similar behavior, and the least reactive side should match the picked data side indicating less or less reactive material. If additional or correctional picking is required, the PC deletes the PRU and FPT entries, and changes the date for the PID instructions to the current date. This will indicate to the PP that picking is required. Comments on the DATA PROCESSING INSTRUCTION FORM will indicate the new work required with notes added by the PC during the last QA procedure. Once the correction PP work is performed, RUNENTRY will be updated with PRU again which will indicate raw data QA procedures are needed again to the PC in the next PCREPORT. If the data passes the QA tests, the PC enters PQA to RUNENTRY which will indicate to the PC in future PCREPORTs that calibration factors are needed for further data processing.

Once the picked data is QAed, calibration factors need to be determined for final data processing: conversion of raw picked data ("P files") to concentration data ("C" files). The techniques for determining appropriate calibration factors was discussed above. The calibration factors are indicated on the DATA PROCESSING INSTRUCTION FORM. The PC indicates that calibration factors have been determined by entering into RUNENTRY CFD (calibration factors determined). This will indicate to the PP that raw data is ready to be converted to concentration data in the next, PPREPORT.

A program (CALCON) which runs on the LSI-11 computer is used to apply the calibration factors to the raw data ("P"-files), and to document which factors were used, who determined them, who is running the program and when, the full names of the compounds (abbreviations are used to identify data fields), and the maximum amplitudes of the raw and final concentration data. Two separate files are produced, the actual concentration data (mmddyC.iit, "C" file) and the documentation (mmddyK.iit, "K" file). The resulting files are listed, and the data is plotted for final QA with PLOCON, a plotting program using GIGI graphics and the LSI-11. These are retained in the run folder. The PP indicates that the CALCON program was run by entering CRU. This will indicate to the PC that concentration files are ready for final QA in the next PCREPORT.

The QA procedure for the final concentration data varies with the complexity of the experiment and the chemical species. The first checks however are to look at the documentation file ("K" file) and the DATA PROCESSING INSTRUCTION FORM to be sure that the desired calibration factor(s) was actually applied. The PLOCON plot is inspected to determine if the resulting data is reasonable and consistent with the other experimental data and the indicated target conditions on the RUN SHEET. If the concentrations of the initial conditions are far from the target conditions, a reasonable explanation must be found. Often the RUN SHEET, REMARKS FILE printout, or the INSTRUMENT CHECKLIST will indicate problems which could explain the discrepancies. Usually resulting data is not more than 25 percent from the target conditions.

If the concentration data is for a standard HC mixture, a compositional analysis should conform well with the known composition. An option of the CALCON program is to produce files which are readable by a computer program (HCANAL) for compositional analysis. In some cases where several experiments are performed with a similar mixture, the concentration data for the initial conditions for all the experiments are entered into a LOTUS spreadsheet for relational composition analysis. Calbration factors should result in data which when analyzed yields a consistent composition if indeed a similar mixture was used throughout the program. QA procedures may indicate that the calibration factors are not reasonable or that the raw data is invalid. See the discussion above for determination of calibration factors. Invalid data may require special processing, or a decision that the data is not processable (BAD). Once QA procedures are successfully performed, RUNENTRY is updated with CQA (concentration data QA performed). The "C" and "K" files are backed-up on floppies. If new factors are needed, the CRU is deleted and the CFD date is updated. New factors are indicated with explanations on the DATA PROCESSING FORM.

Once the final QA procedures are completed, the "C" and "K" files are transfered from the LSI-11 to the VAX (RUNENTRY F2V) to await merging with the DVM data and the documentation, to form the final segmented data file for distribution. The "P", "C", and "K" files are backed up on VAX magnetic tape. The RUN_CAL_USED database is updated with the calibration factors used in data processing. Initial conditions are updated in RUNENTRY in the general section and RUNSUMMARY.

## Documentation Processing

Documentation is associated with all phases of the experiment; recorded on many sources. Much is needed only to process the data. Some documentation data however is processed to be included with the final data files. Calibration factor documentation is processed as the data is processed ("K" file, see discussion above). Some other documentation however is needed, which increases the value of the resulting final data.

A general documentation file is produced in addition to the concentraion data files (`mmddyy.DOC`). It becomes the first part of the final segmented data file. Its purpose is to convey all information with the data file itself. required to describe the experiment, and data which might be useful to photochemical modelers. The processing flowchart is indicated in Figure 23. The `RUNENTRY` events flowchart is shown in Table 18.

18

### Documentation Steps

```
                   DOCUMENTATION data processing steps
Pers     Step                    Meaning
----     ---------------------   -----------------------------------
PC       SUN : Run sum done      DVN, Instrument, and Raw Quality Combined.
CT       D2V : Doc  to VAX       Documentation transferred to VAX
PC       DQA : Doc QA            Documentation Quality Assurance
```

## General Documentation Form

A five page paper form called `General Documentation` is used throughout all stages of the data processing. All documentation needed to be included in the final general documentation file is recorded on this form as data are processed. In addition the form includes checklists and formulas used to arrive at a general quality index that is specified in the final documentation file. An example form is included in Appendix E.

## General Description and Purpose of Experiment

The first part of the general documentation file is the experimental run date which is the primary identifier of an experiment. A general description of the experiment follows. The purpose of the experiment is included if it is not clear from the description. Results are sometimes added if a specific comparison was being made.

## Initial Conditions

The initial conditions of the experiment are listed next. Concentrations for each

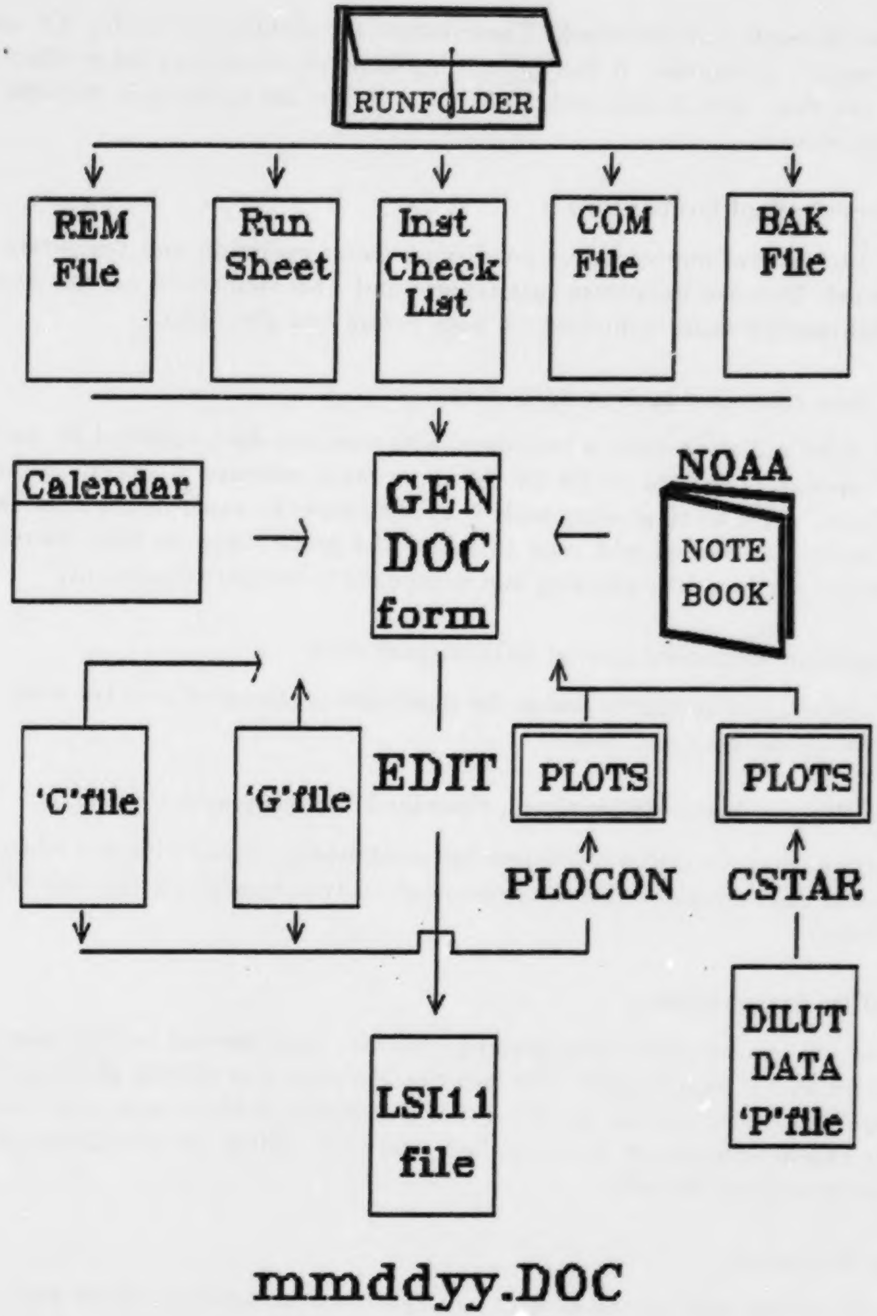

RUNFOLDER
REM File
Run Sheet
Inst Check List
COM File
BAK File
Calendar
GEN DOC form
NOAA
NOTE BOOK
'C'file
'G'file
EDIT
PLOTS
PLOTS
PLOCON
CSTAR
LSI11 file
DILUT DATA 'P'file
mmddyy.DOC

**Figure 23.** Documentation Processing Flowchart (Computers and Files)

species for each side are listed. These values are obtained from the "G" and "C" files, usually at sunrise. If the initial conditions are from data taken after sunrise then the data time is reported. Initial conditions are updated in RUNENTRY in the general section.

## Meteorological Conditions

Next the general meteorologial conditions (solar radiation and temperature) are indicated. Detailed data from NOAA reports and TSR stripcharts are the basis for a general ranking value computed for both before and afternoon.

### *TSR data compared against RDU data*

Total solar radiation data is compared with the NOAA data collected at the nearby RDU airport. The data profile for the experiment recorded at the site is inspected for "holes". A 1 to 10 grading scale is used to rate the experiments solar radiaion. The holes are counted and used to assess the grade value for both morning and afternoon portions (the morning sun is thought to be more important).

### *Temperature compared against RDU airport data*

The temperature at sunrise and at the maximum is compared with the RDU airport data for consistency and listed.

## Data Times, Data Exceptions, Special Problems and Concerns

The times that the initial conditions are established, sunrise time and when the experiment ends are given. Data exception are listed. Special problems and concerns are listed.

## Quality Assessment

An overall quality assessment grading scale has been devised to help compare the large number of experiments. The index ranges from 0 to 10 with 10 being a perfect experiment. Although the assessment of the quality index is somewhat subjective, many characteristics can be quantified relatively. There are five categories which are each weighted equally.

### *Solar Radiation*

For the earlier years of the dataset sun light was the principle factor used for representing run quality. Starting in 1981 more formal methods were developed: a formula which would grade the sunlight quality more consistently but with the same general techniques used earlier: a) the percent of possible solar radiation measured for the day. b) the number "holes or dips" in the radiation profile, and c) morning fog or haze. The earlier sunlight profile of the day is usually considered more import than the post solar noon portion. Therefore the first half of the day is weighted 70of the total quality index. Meteorological data obtained at a local major airport (RDU) lists percent of possible sun data which has been found to correlate well with observed solar profiles and is used to establish the base index value: 90 percent is converted to a quality index of "9". Then "holes" (25 percent or more attenuation of expected intensity) are divided and counted into three classes: 15, 30 and 60 minute duration. Index units are subtracted for each "hole" weighed by duration class.

### *Target Conditions Established*

There are three general areas of concern: a) whether target conditions were obtained, b) whether the internal (one side consideration) and external ratios (two sides compared) for each key condition parameter were obtained, and c) whether the experimental conditions are quantifiable or verifiable.

The base sub-index is set at "10". One index unit is deducted for each 20 percent error from the absolute target condition desired. Very often with the dual smog chambers it is the relative ratios of the initial component concentrations that is more important. There are two types of relative comparisons which are made: the ratios of components to each other within a mixture and the ratios of components in two different mixtures (side by side comparison). If a mixture is used, the relative fractions of components often needs to be carefully established. Very often the initial condition of interest is a matched HC to NOx ratio. One index point is deleted for each 5 percent error from the target relative composition.

Usually initial conditions are verifiable analytically. When an analytical techniques fails or a sample is not taken before the beginning of an experiment, other techniques may have to be used to establish or estimate the initial conditions. Direct injection of neat liquids or gases are often used as a calibration technique and therefore can be used as a second best estimate of initial conditions. If a component of a commonly used mixture is not directly analytically monitored for a particular experiment, its concentration can be estimated from the concentrations of the other mixture components and relative composition data. However these techniques are less than ideal and two index units are deleted from this quality category for each compound not verified by an analytical technique.

### *Analytical Support*

Analytical support is not always available for all species for all runs: techniques sometimes fail during an experiment. The base index is set at "10" and index points are deleted weighed by importance of the species or physical data not measured.

### *Chamber Conditions*

Chamber conditions can have a major impact on experimental results. Important parameters include: a) condensation on walls, b) dilution rate, and c) hours of venting before the experiment. The base index is set at "10".

Condensation observed on chamber walls is noted by the operator starting the experiment. One index point is deleted if condensation is observed on both chambers. Chamber driers do not always operate well and sometimes one side may be dried better than the other resulting in condensation in one side only. Two index units are deleted for this situation.

Dilution rate is usually monitored by use of inert tracers such as CCl4. A exponential least-squares fit analysis yields the dilution rate (necessary for proper modeling) for each chamber. The quality index is deleted by one if the dilution rates differ by more than 20 percent. Additional points are deleted proportionally for dilution rates exceeding the normal dilution rate of 1.5 * 10-4 min-1. The index is deleted by two if the dilution rate is not quantifiable (incomplete of poor tracer data). The quality index is deleted by one if the dilution rate is high or irregular from windy conditions. Dilution rates are normally well matched and less than 10 percent per ten hours.

Two hours of venting will eliminate observable concentrations of chamber pollutants. Regular experimental protocol requires that each run by preceded with at least six hours of venting. Three index points are deleted if less venting time is used.

### *Overall Value—Need*

Other major aspects of an experiment are overall usefulness and value. Many experiments are conducted to satisfy questions requiring immediate attention or special effort. Often these experiments are difficult to conduct; the experimental quality may be less than desired but nevertheless contributes usefull information which may be otherwise impossible to obtain. These experiments may be supportive of other experiments. This category is used to adjust the quality index to reflect these experimental needs.

## Documentation File Production

When all of the documentation information has been collected and the GENERAL DOCUMENTATION form has been filled out, the PC updates RUNENTRY with the SUN event. This will indicate to the CT that documentation information is ready to be moved to the VAX11/780. The CT uses a template file and a text editor. When the documentation file is produced, the CT updates RUNENTRY with the D2V event. This indicates to the PC in the next PCREPORT that the documentation file is ready for final QA. The file is listed and stored in the RUNFOLDER.

The listed documentation file is compared with the GENERAL DOCUMENTATION form to be sure that at least the information was correctly transfered. The documentation information is checked one last time with general experimental results: plots of the experimental data are compared with the initial conditions for consistency of relative reactivity. The stated initial conditions and the data plots should be checked for agreement. The quality indices for sunlight should be compared with the light plots for reasonableness. The general run quality index should be checked for overall reasonableness having read the documentation and looked at the data plots. If it is low, the reasons should be apparent in the documentation (*e.g.*missing data, chamber condensation present, or poor sunlight).

When the QA criteria are satisfied, the PC updates RUNENTRY with the DQA event. The GENERAL section of RUNENTRY is updated with the final initial conditions and the quality index value. This is usually the last step before producing the final segmented file.

## Final Segmented File Production

When all data processing tasks are completed, the files are moved to the VAX11/780. The files are merged together with a procedure called FINALMRG which follows a prescribed order. An ASCII labeled tape is made. Plots are made from the segmented file as a QA step: if the format is incorrect the plotting programs will probably not be able to read the file. The file is listed and inspected. The RUNENTRY event flowchart is shown in Table 19.

## Table 19.

## Final Segmented File Production Steps

```
FINAL FILE data processing steps
Pers     Step                    Meaning
----     ---------------------   -----------------------------------
CT       MR3 : Merged 3 sect     Merge pieces to final file
CT       ALT : Files to tape     Ascii labeled tape made
CT       FPC : Final plot done   Correct conc plot made
PC       FQA : Final QA          Final Quality Assurance
PC       NTB : Not to be proc
PC       BAD : Stop processing   Something is wrong with this data
```

## Security of Data

There are three basic activities to enhance data security: inventory, retention of original data to restricted areas, and maintaining several backup copies of all data in different locations. All data are under lock at night.

### Inventory

Before anyone is allowed to work with the run folder contents, a run folder inventory is performed which documents all data and forms. This helps assure that no data or documentation is lost.

### Retention of Data

All original data, both paper and electronic files are retained. Paper formated data (all stripcharts, forms) are not allowed out of the office.

### Backup of Data

Multiple copies of data are maintained in several formats in several locations. Backup copies of raw and final data on floppies on the IBM PC are kept in several locations. Lotus worksheet files are backed up in two locations. Hardcopy (printouts) of worksheet formulas using a spreadsheet AUDITOR is kept. Backup copies of raw and final data on LSI11/23 computers are maintained in several locations, including: raw data and processed data sets backed up on two diskettes, processing programs (sources) backed up on two diskettes, and whole image harddisk backup of LSI11/23. Backup copies of final data are maintained on the VAX and further backed-up on tapes of VAX files. Frequent printouts of of data in all stages of processing ("P"-, "C"-, and "K"-files) and plots are kept in runfolders and in notebooks.

# 5

# Segmented Data File

This section describes the final segmented data file used for distribution of the experimental results.

## General Description

All of the data for a run are stored in a single file. This includes: documentation including the calibration information; the continuous instrument data, every 4-minutes, alternating on chamber sides in physical units; and the gas chromatographic instrument data given in concentration units for each side of the chamber for each instrument approximately every 30 minutes.

# File Formats

No record exceeds 80 columns (data is in "card image") form. The general lay out of the file is:

```
DOCUMENTATION  segment <starts with first record>
     General documentation section
88888 <documentation section terminator>
     first instrument documentation ''K-file'' section
88888 <documentation section terminator>
     second instrument documentation ''K-file'' section
88888 <documentation section terminator>
  ...        .....
88888
     last instrument documentation section
88888 <terminator>
     DVM data documentation section
99999    <END OF DOCUMENTATION SEGMENT>
     DVM Data, up to 3 ''cards'' per time
99999    <END OF INSTRUMENT DATA SEGMENT>
     First instrument data, up to 3 ''cards'' per time
99999    <END OF INSTRUMENT DATA SEGMENT>
     Second instrument data
99999    <END OF INSTRUMENT DATA SEGMENT>
  ...        .....
99999     <END OF FILE>
```

An example segmented data file is shown in Table 20.

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## Table 20. Example Segmented Data File

```
                   GENERAL DOCUMENTATION

RUNDATE: OCTOBER 04, 1983

RUNTYPE: AUTO

RUN DESCRIPTION: COMPARISON OF REACTIVITY OF EXHAUST
FROM DIRECT INJECTION FROM DODGE CHARGER IN HIGH IDLE
WITH SYNTHETIC AUTOEXHAUST.

RESULTS: TWO SYSTEMS RESULTED IN SIMILAR REACTIVITY

INITIAL CONDITIONS:          BLUE          RED
DODGE CHARGER                0.0           2.587
SYNTHETIC EXHAUST NMHC       2.190         0.0
NO                           0.214         0.215
NO2                          0.037         0.039
.
.
.
88888
04-OCT-83                                  GENERATED ON 19-MAR-84
SY:OCO43K.C1G       .C1G
PICKED DATA ENTERED BY JEFFREY HOFFNER
CALIBRATION FACTORS APPLIED BY CHARLES
TOLUENE                          2.912000E-01   PPMC/IN     2     KGS
ETHYLENE                         9.020000E-02   PPMC.IN     2     KGS
.
.
NAME ABBREVIATIONS - SAME ORDER AS IN DATA
TOLUENE   IS TOLUENE                   MAX A:   1.5610 MAX CON:   0.4546
ETHYLENE  IS ETHYLENE                  MAX A:   4.9164 MAX CON:   0.4435
.
.
```

## Table 20, cont. Example Segmented Data File

```
88888
04-OCT-83                                        GENERATED ON 13-MAR-84
SY:OCO43K.C2G       .C2G
PICKED DATA ENTERED BY JEFFREY HOFFNER
CALIBRATION FACTORS APPLIED BY JEFFREY HOFFNER
ETHANE                                1.498000E-01   PPMC/IN      2     KGS
PROPYLENE                             7.307000E-01   PPMC/IN      2     KGS
.
.
NAME ABBREVIATIONS - SAME ORDER AS IN DATA
ETHANE    IS ETHANE                              MAX A:   0.2014 MAX CON:   0.0302
PROPYLENE IS PROPYLENE                           MAX A:   0.1311 MAX CON:   0.0958
.
.
88888
.
.
.
88888
USER DOCUMENTATION FOR RUN 831004
.
.
CALIBRATION FACTORS USED:
SPECIE
 TIME     INTERVAL  BEGINNING    GAIN     ENDING  BEGINNING    OFFS     ENDING
                       GAIN      SLOPE     GAIN     OFFSET     SLOPE    OFFSET
  HR        HR                   HR-1                          HR-1
03G
  2.500   15.500      1.01380   0.00000   1.01380   0.00000   0.00000   0.00000
 18.000    6.000      0.00000   0.00000   0.00000  -9.99999   0.00000  -9.99999
.
.
END OF PROGRAM DOCUMENTATION
99999
YYMMDDHHMM    U     S     03G        NOG        NOXG       NO2G       DPG       CTMP
    LTMP     TSR          UV
8310040500    1    7R    0.0008     0.0864     0.1138     0.0237    50.0450   56.8300
   58.6810  -0.0046     -0.2439
8310040504    1    3B    0.0196    -0.0022    -0.0007     0.0001    56.6496  -60.5560
   21.6880  -0.0062     -0.2439
.
.
```

### Table 20, cont. Example Segmented Data File

```
.
.
8310041704    1   3B    0.5787   -0.0012    0.0513    0.0507   72.7266  -60.5120
   20.5120    0.1592   11.7073
8310041708    1   7R    0.5508   -0.0013    0.0578    0.0573   64.7658   83.3620
   81.3040    0.1376   10.2439
99999
YYMMDDHHMM    USER SIDE      GENERATED ON 19-MAR-84
2,4,4 TRI TOLUENE   ETHYLENE  N-BUTANE  TRANS-2-B ISOPENTAN N-PENTANE ACETYLENE
8310040625    1    B
   0.2266    0.4546    0.4435    0.0877    0.0366    0.1339    0.0000    0.0905
8310040655    1    R
   0.1868    0.2580    0.2248 -999.0000    0.0459    0.1195    0.0634    0.2332
.
.
8310041455    1    R
   0.1439    0.1573    0.0890 -999.0000    0.0000    0.0828    0.0340    0.1672
8310041525    1    B
   0.1821    0.2514    0.1300    0.0688    0.0000    0.0921    0.0000    0.0000
99999
YYMMDDHHMM    USER SIDE      GENERATED ON 13-MAR-84
ETHYLENE  ETHANE    PROPYLENE
8310040625    1    B
   0.4522    0.0093    0.0952
8310040655    1    R
   0.4097    0.0238    0.0958
.
.
8310041525    1    B
   0.1603    0.0086    0.0000
8310041555    1    R
   0.2675    0.0260    0.0000
99999
```

## ANSI Tape File Format

The segmented data files are written one file after the other onto 1/2 inch wide industry standard magnetic tape at a density of 1600 bits per inch.

We have adopted the American National Institute of Standards (ANSI) standard labeled tape format. This format is supported by a wide variety of computers including most mini-computers, and IBM. An advantage of a labeled tape is the "directories" of the tape contents can easily be created without having to list the data.

Individual records of the files are collected together into a "block" of records before being written to the tape. They can appear on the tape in one or two forms: fixed length, blocked rocords, or variable length, blocked records. The default value is fixed length blocked records with a record size of 80 bytes and a block size of 2000 bytes. For variable length records, the records are between 5 bytes and 84 bytes, and the block size is 2048 bytes.

Figure 24, Figure 25, Figure 26, Figure 27, Figure 28, Figure 29, Figure 30, Figure 31, and Table 21, Table 22, Table 23, and Table 24 explain the details of the ANSI tape format as an aid in reading the tape. Volumn identifiers on the ANSI tape (in the VOL1 label field are UNC001 to UNC010 depending upon the release.

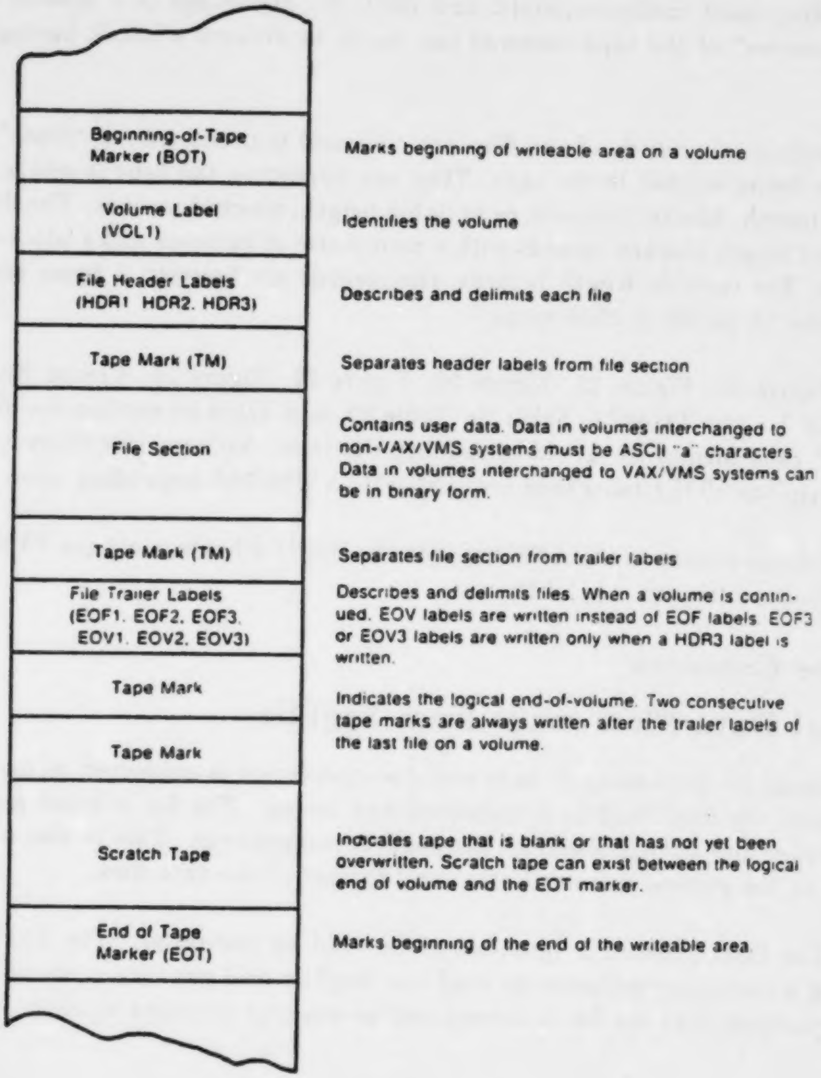
File identifiers on the ANSI tape (in the HDR1 label format) are YYMMDD.SEG for the year, month, day of the run.

## Tape Contents

## Final Data Plots made from SegFile

Although all processing of data and documentation is subjected to many QA procedures, the final SegFile is inspected and tested. The file is listed and inspected for order and completeness of the SegFile components. This is also a last chance look at the general documentation and format of the data files.

The final product is intended to be read by computer. The final QA test is using a computer program to read the SegFile and produce plots of the data to demonstrate that the file is correct and to examine the data visually.



| | |
|---|---|
| Beginning-of-Tape Marker (BOT) | Marks beginning of writeable area on a volume |
| Volume Label (VOL1) | Identifies the volume |
| File Header Labels (HDR1, HDR2, HDR3) | Describes and delimits each file |
| Tape Mark (TM) | Separates header labels from file section |
| File Section | Contains user data. Data in volumes interchanged to non-VAX/VMS systems must be ASCII "a" characters. Data in volumes interchanged to VAX/VMS systems can be in binary form. |
| Tape Mark (TM) | Separates file section from trailer labels |
| File Trailer Labels (EOF1, EOF2, EOF3, EOV1, EOV2, EOV3) | Describes and delimits files. When a volume is continued, EOV labels are written instead of EOF labels. EOF3 or EOV3 labels are written only when a HDR3 label is written. |
| Tape Mark | Indicates the logical end-of-volume. Two consecutive tape marks are always written after the trailer labels of the last file on a volume. |
| Tape Mark | |
| Scratch Tape | Indicates tape that is blank or that has not yet been overwritten. Scratch tape can exist between the logical end of volume and the EOT marker. |
| End of Tape Marker (EOT) | Marks beginning of the end of the writeable area. |

Figure 24. Basic Layout of a VAX/VMS ANSI Labeled Volume

Labels and Components Supported by VAX/VMS

| Symbol | Meaning | Symbol | Meaning |
|---|---|---|---|
| BOT | Beginning-of-tape marker | EOV3 | Third end-of-volume label |
| EOF1 | First end-of-file label | HDR1 | First header label |
| EOF2 | Second end-of-file label | HDR2 | Second header label |
| EOF3 | Third end-of-file label | HDR3 | Third header label |
| EOT | End-of-tape marker | VOL1 | Volume label |
| EOV1 | First end-of-volume label | TM | Tape mark |
| EOV2 | Second end-of-volume label | TM TM | Double tape mark indicates an empty file section or the logical end-of-volume |

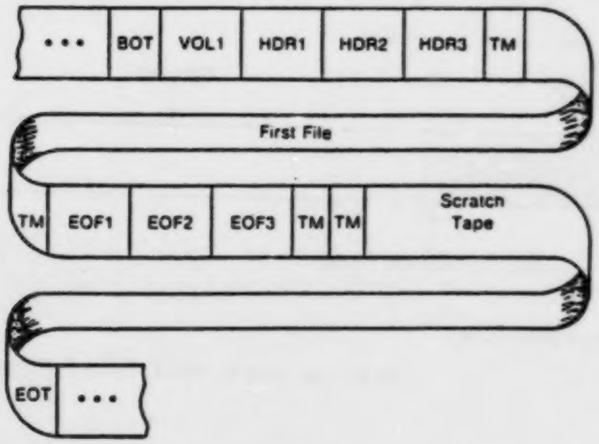
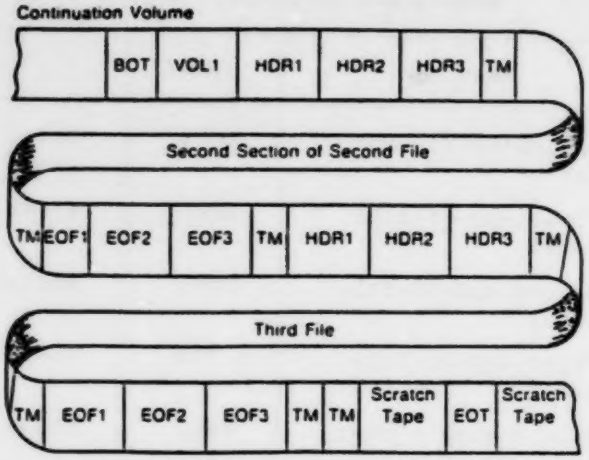
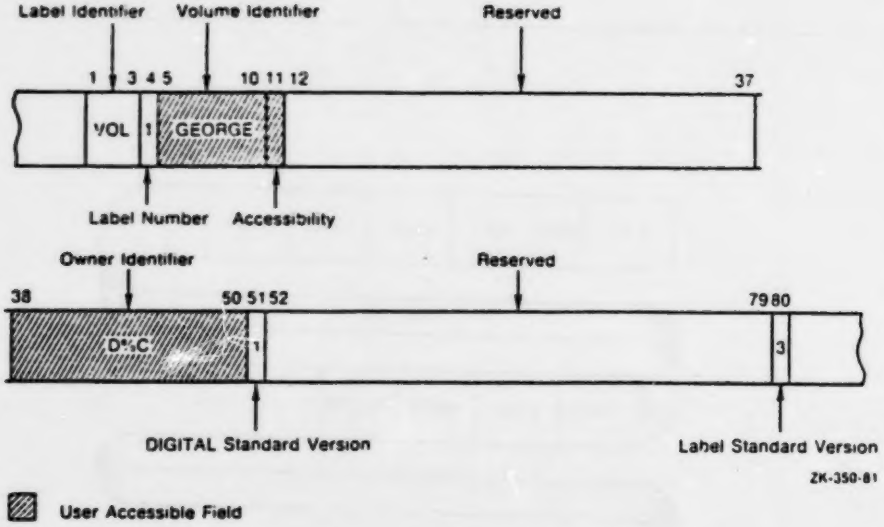

...
BOT
VOL1
HDR1
HDR2
HDR3
TM
First File
TM
EOF1
EOF2
EOF3
TM
TM
Scratch Tape
EOT
...

**Figure 25.** Single File/Single Volume Configuration


Continuation Volume
BOT
VOL1
HDR1
HDR2
HDR3
TM
Second Section of Second File
TM
EOF1
EOF2
EOF3
TM
HDR1
HDR2
HDR3
TM
Third File
TM
EOF1
EOF2
EOF3
TM
TM
Scratch Tape
EOT
Scratch Tape

Multifile/Multivolume Configuration


Label Identifier
Volume Identifier
Reserved
1
3
4
5
10
11
12
37
VOL
1
GEORGE
Label Number
Accessibility
Owner Identifier
Reserved
38
50
51
52
79
80
D%C
1
3
DIGITAL Standard Version
Label Standard Version
ZK-350-81
▨ User Accessible Field

VAX/VMS ANSI VOL1 Label Format

**Figure 26.**

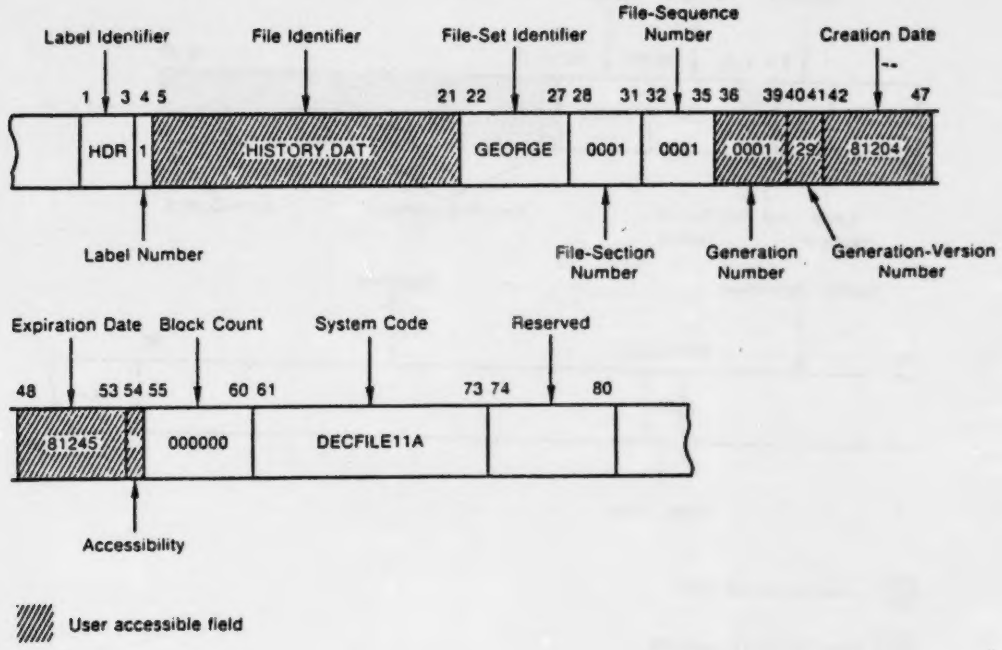

Label Identifier
File Identifier
File-Set Identifier
File-Sequence Number
Creation Date
1
3 4 5
21 22
27 28
31 32
35 36
39404142
47
HDR
1
HISTORY.DAT
GEORGE
0001
0001
0001
29
81204
Label Number
File-Section Number
Generation Number
Generation-Version Number
Expiration Date
Block Count
System Code
Reserved
48
53 54 55
60 61
73 74
80
81245
000000
DECFILE11A
Accessibility
User accessible field

**Figure 28.** HDR1 Label Format

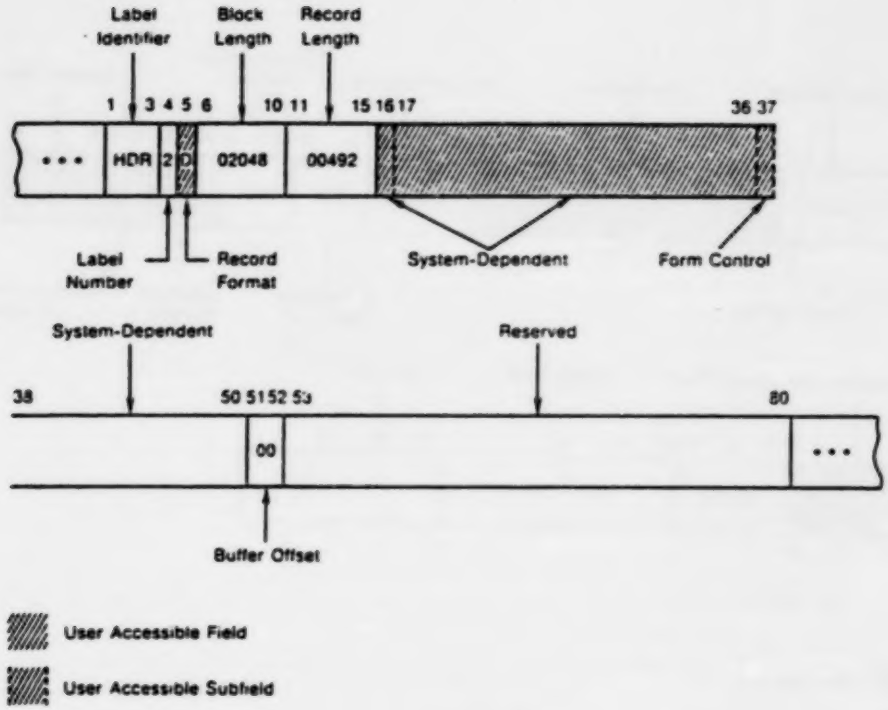
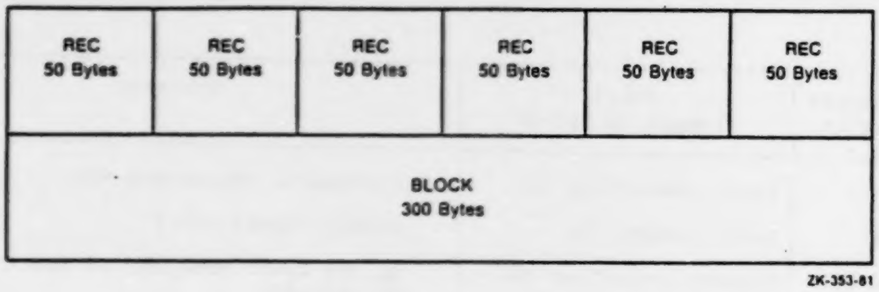
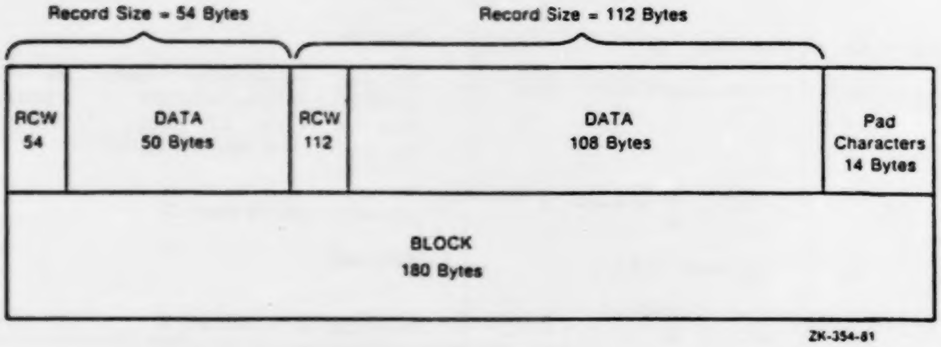

Label Identifier
Block Length
Record Length
1
3
4
5
6
10
11
15
16
17
36
37
• • •
HDR
2
D
02048
00492
Label Number
Record Format
System-Dependent
Form Control
System-Dependent
Reserved
38
50
51
52
53
80
00
• • •
Buffer Offset
User Accessible Field
User Accessible Subfield

**Figure 29. HDR2 Label Format**


REC
50 Bytes
REC
50 Bytes
REC
50 Bytes
REC
50 Bytes
REC
50 Bytes
REC
50 Bytes
BLOCK
300 Bytes
ZK-353-81

Blocked Fixed-Length Records


Record Size = 54 Bytes
Record Size = 112 Bytes
RCW
54
DATA
50 Bytes
RCW
112
DATA
108 Bytes
Pad
Characters
14 Bytes
BLOCK
180 Bytes
ZK-354-81

Variable-Length Records

**Figure 30.** Blocked Fixed-Length Records

## Table 21. VAX/VMS ANSI VOL1 Label

| Character Position | Field (length in bytes) | Contents |
|---|---|---|
| 1 - 3 | Label Identifier (3) | Alphabetic characters VOL |
| 4 | Label Number (1) | Numeric character 1 |
| 5 - 10 | Volume Identifier (6) | Volume label consists of ASCII "a" characters. |
| 11 | Accessibility (1) | Volume accessibility; provides compatibility with some non-VAX/VMS systems. A space, the VAX/VMS default, indicates no restrictions. To write any ASCII "a" character in this field, use /LABEL=VOLUME_ACCESSIBILITY with the INITIALIZE command. Any character but a space indicates the /OVERRIDE qualifier must be used with the INITIALIZE and MOUNT commands. |
| 12 - 37 | Reserved (26) | Spaces |
| 38 - 50 | Owner Identifier (13) | Volume ownership set by the INITIALIZE/PROTECTION command. The contents of this field are used for volume protection |
| 51 | DIGITAL Standard Version 1 | Numeric character 1 |
| 52 - 79 | Reserved (28) | Spaces |
| 80 | Label Standard Version 1 | Numeric character 3 |

Table 22. First File Header Label (HDR1) Fields

| Character Position | Field (length in bytes) | Contents |
|---|---|---|
| 1 - 3 | Label Identifier (3) | Alphabetic characters HDR |
| 4 | Label Number (1) | Numeric character 1 |
| 5 - 21 | File Identifier (17) | A user-supplied file name and file type |
| 22 - 27 | File-Set Identifier (6) | Same as the file-set identifier of the first file on the first volume, whether single or multivolume configuration |
| 28 - 31 | File-Section Number (4) | Numeric characters starting at 0001 and incrementing by 1 for each additional volume with respect to the first volume on which the file begins |
| 32 - 35 | File-Sequence Number (4) | File number within the volume set for this file; consists of numeric characters, starting at 0001 that indicate the position of this file with respect to the first file of the set |
| 36 - 39 | Generation Number (4) | Numeric characters that indicate the unique generation of a file |
| 40 - 41 | Generation-Version (2) Number | Numeric characters that indicate the version of a particular generation of a file |
| 42 - 47 | Creation Date (6) | System stores the date in the Julian format (#YYDDD)[1]; the default is the current date |
| 48 - 53 | Expiration Date (6) | User specified Julian date (#YYDDD)* or default is the creation date, indicating file expires immediately |
| 54 | Accessibility (1) | File accessibility; provides compatibility with some non-DIGITAL systems. A space (used by DIGITAL systems) indicates no restrictions. Any character but a space indicates the /OVERRIDE qualifier must be used at mount time for the user to access this file. |
| 55 - 60 | Block Count (6) | Always 000000 for the HDR1 label |

1. The number sign (#) in the Julian format represents a space.

(continued on next page)

## Table 22. (Cont.): First File Header Label (HDR1) Fields

| Character Position | Field (length in bytes) | Contents |
|---|---|---|
| 61 - 73 | System Code (13) | Identifies the file system that created the file. DEC, the 3-character constant, occupies positions 61 through 63, followed by the name of the file system; DECFILE112 indicates VAX/VMS Version 1.6 and earlier, and DECFILE11A indicates VAX/VMS Version 2.0 and later. |
| 74 - 80 | Reserved (7) | Spaces |

## Table 23. Second File Header Label (HDR2) Fields

| Character Position | Field (length in bytes) | Contents |
|---|---|---|
| 1 - 3 | Label Identifier (3) | Alphabetic characters HDR |
| 4 | Label Number (1) | Numeric character 2 |
| 5 | Record Format (1) | Character definition:<br>F fixed-length<br>D variable-length<br>The S for spanned record format is returned as an undefined format when processed by VAX/VMS[1] |
| 6 - 10 | Block Length (5) | Five numeric characters specifying the maximum number of characters per block |
| 11 - 15 | Record Length (5) | Numeric characters indicating the record length for fixed-length records or the maximum record length for variable-length records |
| 16 | System-Dependent (1) | In VAX/VMS Version 2.1 and later versions, this field contains a space indicating the VAX-11 RMS attributes are in the HDR3 label<br>For VAX/VMS Version 2.0 and previous versions, this field does not contain a space but contains the first byte of the VAX-11 RMS attributes, indicating the VAX-11 RMS attributes are in the HDR2 label |

1. To process undefined records properly, the user must know what the original format of the records was. Only logical I/O can be used to process undefined record formats.

(continued on next page)

Table 23. (Cont.): Second File Header Label (HDR2) Fields

| Character Position | Field (length in bytes) | Contents |
|---|---|---|
| 17 - 36 | System-Dependent (20) | Spaces available for future use. For VAX/VMS Version 2.0 and earlier, this field contains the VAX-11 RMS attribute in binary format |
| 37 | Form Control (1) | Defines the carriage control applied to the records within a file, as follows:<br>A First byte of record contains FORTRAN control characters<br>M Record contains all form control information<br>Space Line feed/carriage return will be inserted between records (default) |
| 38 - 50 | System-Dependent (13) | Spaces available for future use. For VAX/VMS Version 2.0 and earlier, this field contains the VAX-11 RMS attributes in binary format |
| 51 - 52 | Buffer Offset (2) | The numeric characters 00 |
| 53 - 80 | Reserved (28) | Spaces |

Table 24. Third File Header Label (HDR3) Fields

| Character Position | Field (length in bytes) | Contents |
|---|---|---|
| 1 - 3 | Label Identifier (3) | Alphabetic characters HDR |
| 4 | Label Number (1) | Numeric character 3 |
| 5 - 68 | VAX-11 RMS Attributes (64) | Files-11 record attributes that override information in fields of the HDR2 label |
| 69 - 80 | System-Dependent (12) | Spaces |

# 6

# Summary of QA

## Summary of Calibration and Data QA

- 3 NBS traceable standards for NO were used in this project
- the three standards agreed at 3 concentration levels to within an average of 2.3 percent of each other
- 8 HC tanks and precision liquid chamber injections were used as calibration sources in this project; two of the HC tanks were NBS tanks from an RTI multi-year comparison study
- the four principle HC tanks, validated with the RTI tanks and liquid chamber injections, agreed to within an average of 1.6 percent of each other; and agreed to within an average of 3.7 (std dev 1.8 percent) percent to the manufacturers specified concentration values
- HC calibration factors show very little or no trend in instrument sensitivity during the experimental season; the relative standard deviation from the mean calibration factors for the principle species used in this project ranged from 5 to 14 percent with an average of 9.9 percent (std dev 2.2 percent).
- computer spreadsheets were used to adjust calibration factors (within observed "noise" range) to maintain consistency of experimental initial conditions composition produced from fixed composition (pressurized gas tank and liquid mixture) HC sources used in this project.
- two pressurized tanks of HC mixtures were used to produce the experimental initial conditions of the lower molecular weight compounds assuring consistent composition and initial concentration throughout the experiment series

- one of the principle HC source tanks for the experimental program (UNCMIX, a component of the synthetic urban mixture) is certified to 2 percent
- a liquid mixture of the higher molecular weight compounds was prepared and used throughout the program permitting one large neat injection to be made with 1 percent syringes to establish the experimental initial conditions: assuring consistent composition and initial concentration throughout the experiment series
- a multi-computer-based data acquisition and data processing system incorporated into a QA program which monitors every step of data generation and processing is utilized to minimize risk of human error and maximize accuracy and overall data quality.

## List of QA Steps

This section lists all specific QA steps performed.

### Before Runs

- review progress and schedule of experiments from work plan:
  - do experiments to date make sense? are they consistent?
  - do they indicate new experiments or other immediate needs?
  - are data for these experiments good enough or must they be rescheduled?
- check site status and weather report
- match highest priority experiment with immediate site capabilities
- fill out run sheets and instrument checklists
- use site checkout lists
- perform instrument checkout and calibration

### After Run-Experiment Logging

- PC phone call to site and update calendars:
  - verify general quality of run and conditions
  - reschedule?
- use "pack-up" inventory checklist at site
- check calendar for transfering data to floppies at site

- perform runfolder inventory
  - verify proper and complete documentation from site
  - verify complete data from site
- RUNENTRY - log experiment; store folder in office bookcase by date
- calibration folders - store in office bookcase by date
- CALENTRY - log any calibration performed
- calendar, run folder/RUNENTRY, fastplot in notebook check:
  - were runfolder and computer data transfered to data processing office?
  - successfully ?

## During Calibration

- planning:
  - what species will be measured; what calibration sources needed?
  - frequency?
  - technique?
  - documentation required?
  - procedure for transfering calibration data to dpo?
- identify standards and perform cross comparison:
  - check standards consistency
- CALENTRY - calibration log and processing status database:
  - during run log-in: check instrument checklist for calibrations performed or check for presence of calibration folder:
  - log calibration data in calentry
- routinely check CALENTRY:
  - check that all have been given processing instructions
- check documentation QA while giving processing (pick) instructions:
  - verify proper and complete documentation from site
- inspect calibration data stripchart for appropriate appearance
  - mark peak ids and chromatograms to pick
- routinely check CALENTRY:
  - check that all have been digpicked

- after `DIGPIK` inspect picked raw data on computer - compare with stripchart data
- routinely check `CALENTRY`:
  - check that all are run through `CALFAC`
- run `CALLOK`:
  - check report lists and plots to display results for representative compounds for early QA to identify any problems
- check `DTR HCCAL` database:
  - generate `HCCAL` report and scan entire report:
  - observe large variations and problems
- run `CALANA`: final check and statistical analysis
- during determination of calibration factors for data processing: does calibration result in meaningful data?

## During DVM Data Processing

- calendars and `CTREPORT` inspection:
  - are there data files missing?
  - new files to be unpacked?
- documentation comparison:
  - run sheet, instrument checklist, remarks file: what were target conditions?
  - any problems recorded?
- inspect stripchart:
  - were target conditions achieved (within calibration uncertainty)?
  - documentation complete? recorder settings, side, time for all pens?
  - does data make sense? are there unexplained problems? missing or noisy data?
- `FASTDV` plot and comparison with stripchart data
- `AUTOCAL` strip (see cal)
- `AUTOCAL` report:
  - did `AUTOCAL` data get processed?
  - any problems or large variation?
- run `DVMFIX`:

  - check that DVHFIX $NO_x$ concentration equals concentration of NO plus $NO_2$ all during experiment
  - check for good zeros
- QA PLOCON plots:
  - can plot file (format good)
  - data plot agrees with original stripchart
  - was data processed properly? correct times, sides, and general magnitude?
  - were holes processed properly?
  - dewpoint data higher than temperature?
  - does temperature data check with RDU airport?

## During GC Data Processing

- PCREPORT from RUNENTRY:
  - instruments needing pick instructions correct?
- documentation comparison:
  - inspect run sheet, instrument checklist, remarks file:
  - what were target conditions?
  - any problems recorded?
- inspect stripchart
  - instrument documentation complete? recorder settings, instrument atten, sides, time?
  - does data make sense? see run sheet:
  - is there missing or noisy data?
  - is data good? worth processing? bad?
  - identify calibrations and mark not to be processed as run data
  - identify compounds, pick start and end time, bad data to be skipped, baselines for peaks
- compare raw data stripchart and picked computer file:
  - is raw (picked) data picked correctly?
- PLOPIC plots (of raw data)
  - does data look reasonable? no side switching, attenuation switching problems?

  - sides id correct?
- after CALCON:
  - perform checks on C- and K-files and plots
- calibration factors and RUNCALUSED:
  - are calibration factors used consistent with others, or if not are they explainable?
- compare K-file with data processing instruction form
  - are the calibration factors used shown in K-file the same as specified in data processing instruction form?
  - are names of species correct?
- PLOCON plots:
  - can plot be made (file format correct)?
  - do plots seem reasonable?
- HCANAL or LOTUS:
  - if HC data for mixture, is composition consistent with known composition?
- run sheet target:
  - is resulting data consistent with target experimental conditions? or expected initial conditions?

## During Documentation Stages

- compare documentation:
  - inspect run sheet, instrument checklist, remarks file, calendars:
    - what were target conditions? any inconsistencies? may need to consult site operators (see run sheet)
    - any problems recorded?
    - special conditions, modifications, or operations performed?
    - missing data? species not measured?
    - how many hours of venting?
    - drying performed? condensation observed in morning?
- inspect stripcharts for notes of injection times or amounts
- check climate data, site temperature and light data:
- inspect data files and plots:

  - how complete is data?
  - explanations available for lost data?
  - reason to communicate this to modelers?
- K-files check:
  - documentation complete?
  - any species co-eluting requiring documentation editing?
- compare original experiment list, general documentation paper form and run ranking formulas, and computer file:
  - is information consistent or explainable?
  - was experiment close to target? if not why not?
  - is paper form with general documentation and formulas reduced and transfered correctly to computer file (general doc for segfile)?

## After SegFile Made

- verify file format and contents:
  - by listing file and performing a visual inspection of the contents
  - and by plotting data from file and inspecting plots

# References

1 Smog Chamber Background Reactivity, Part1: The Influence of $NO_x$ from Chamber Walls on Kinetic Computer Models for Air Pollution, submitted for publication

2 Smog Chamber Background Reactivity, Part2: The Influence of Radicals from Chamber Walls on Kinetic Computer Models for Air Pollution, submitted for publication

3 Code of Federal Regulations, Title 40, part 50, subchapter C, Appendix F, pages 568-572.

# A

# Site Checklists

## Checklist For 0900 EDT Site Operator.

As you leave car walk by the red barn and pick up keys. A note pad for listing problems detected in checkout should be used.

### Outside Check

- Walk towards smog chamber on service-gas-tank-house-side of lab. Look at lab door. Are there any messages?
- Listen for Air generator pump running—pull back on metal plates protecting pump and inspect:
  - are pumps upright?
  - do they sound "right"?
- Quick check five service gas tanks (assuming BECKMAN THC is not operational): He, $H_2$ for Carles, $O_2$ for $NO_x$ meter, ethylene for $O_3$ meter, and $Ar/CH_4$ for Varian PAN instrument (generally need minimum of 100 lbs in tank to get through the day). While in the service tank house, check flood lamps mounted on wood chamber platform; if they are on, turn them off.
- Continue walking to BLUE chamber - walk to where manifold goes under chamber. Check service tank $N_2$ for AC driers air circulation valve actuators: secondary meter should show between 15 and 20 lbs and **NOT** higher or it will destroy pneumatic valves: note total lbs in tank and replace (later in the morning) if below 100 lbs.

- Touch heat tapes on BLUE Glass manifold: they should be warm. Inspect for condensation. Look along length of manifold including under chamber for large breaks or condensation. Visually check BLUE circulation fan over injection manifold in chamber: it should be running and turning smoothly.
- Walk to opposite side of chamber and observe venting doors (Make mental note of doors for comparison with run sheet which will be read shortly.
    - If there is no run then chamber is probably venting; all doors should be open and exhaust fan should be on.
    - If a "run" is on-going then in most cases all doors will be shut. Check RED exhaust door and make sure it is closed completely and door motor arm is positioned exactly like BLUE door motor arm.
    - If auto driers (AC system) is operational (one of the circulating fans will be on) then an intake door will be open.
    - If the dehumidifiers were used for drying they should have been removed before injections. If they have not, make note on the runsheet and call PC to determine if the experiment can be continued.
- Visually inspect for condensation both inside and outside the chamber on both sides (RED and BLUE). Rub hand over a large area of one of the side (not end) panels. Note any large drops of water or puddles on the floor of chamber. Note position of center teflon wall separating the chambers. Does it seem to hang more to one side than the other? Are all the fans running? Finally look for general problems such as mud (footprints), bugs, objects (tools, tape, paper towels, etc). in the chamber. Are the glass return and sample manifold intact? If the dehumidifiers were recently removed, were the service panels replaced and seated properly?
- Continue walking around the chamber to the other side back to the injection house and complete inspection of glass (RED) manifold. Feel heat tapes and inspect for condensation, breaks along length including under chamber. Is the RED thermistor laying on the ground?
- Go to BLUE side door in injection tank house. Observe if door is open or closed. It should be closed. Open door to inspect tanks, manifold, and solenoid plugs. Do not touch anything except the RED and BLUE injection lines! Do not turn off any tanks or touch any regulators. You will be coming out again shortly. Check that the RED and BLUE 1/4 inch Teflon injection lines are connected to the glass manifold. Check to see that they are tightly connected. Check to see if ALL computer controlled AC power boxes for solenoids have a plug in it (not including the light brown plastic box used for the WOOD project). They

should also each have a light bulb.

- Close door and go to the other side: open door. Do any of the wires leading over the door catch? Quickly inspect this side of the injection shed for problems. Don't touch anything yet. Don't close any tanks yet. Is there a small wrench for turning off the $NO_2$ tank later? Close the door.
- Go inside the lab on the same side of building. Look up as you enter and notice if the outside floods are on. If they are turn them off with the switch just inside the door as you enter.
- Turn to the right as you enter and head for the $NO_x$ and $O_3$ strip chart. Look and observe if NO and $NO_2$ (or possibly $O_3$) have been injected. Notice approximate concentrations. Are conditions matched (generally)?
- Head for computer console (decwriter). Is the computer and DATCOL up? Are there error messages? Is there a print profile? If not, can you get the time of day from the computer? (Type TIME and return.)

  Are ALL switches in AUTO? Or is there a note saying some should be in MANUAL? Is the 4 minute clock in AUTO?
- Turn around and look for a filled out run sheet for today's run. What was the run today? Look at the command file printout if there is one. What was injected? What tanks were used? Did anything have to be injected or otherwise done manually? Was someone here this morning? See if morning operators name is filled in. Are there any notes on the desk?
- Does $NO_x$ and $O_3$ stripchart make sense compared to information on run sheet? Walk towards Carle GCs. Were injections made? Make quick inspection of chromatograms. Did anything show?
- Go outside to the injection shed (Carle side). Consider the run sheet, command file, $NO_x$ and $O_3$ stripcharts, and GC stripcharts. If injections were scheduled but failed, inspect tanks to see if they were turned on and connected to appropriate solenoids. Were they plugged in? R/B injection lines connected to the glass return manifold? If resulting injections seemed low, check flow rate. (Hastings mass flowmeter reads 8.7 for 10.0 lpm: check with soap bubble flowmeter with $N_2$).
- Once you are finished with the injection shed, turn off all tanks with the main valve. Do not turn off tanks with the regulator. Use a small wrench to close the $NO_2$ tank valve.
- Enter the lab again on the $NO_x$ and $O_3$ side. Go to the DVM and HP clock. Is the DVM scanning? If not, issue immediate command get time from the computer by typing TIME and return. Does the HP clock match? (If not set it

later). Check 4 minute side light. Go over quickly to $NO_x$ and $O_3$ instruments.

- Check $NO_x$ and $O_3$ pressure (20) and vacuum pump pressure (25.5). Check $O_3$ ethylene (15) and rotoball setting. Mark stripchart with current side and time. Does it look like the 4 minute R/B switching valve is operating? Perfect matched injections are almost impossible. If it looks like a perfect match, check the valve and the computer 4 minute switch again. Check that stripchart is marked properly for run date, instrument, stripchart settings, attenuation, *etc.*
- Is the HCHO instrument running? Should it be? Is the sample pump on? Is the rotoball at 4? Is the solutions pump on? Is it drawing solution? Are bubbles running through mixing/reacting chamber (below solutions pump). Check degasser chamber (on right side). It should not be filling up with liquid (a little bit at the bottom is ok). Check each sample line. Look at the HCHO stripchart. Does the signal trace look "right"? Check strip chart zero by pushing down black zero button: it should not be negative. If it is adjust it to about 10% of the chartscale. Adjust HCHO zero if necessary and make note on stripchart.
- Check waste container. Is it too full? Check that stripchart is marked properly for run date, instrument, stripchart settings, attenuation *etc.* Check dewpoint instrument stripchart. Check dewpoint stripchart zero. Mark it as zero check, and mark time and side. Is DP pump on? Is signal trace reasonable? IF there is a difference in dewpoint between the two sides the signal should be a square wave. If it shows a slow response, clean the detector and rebalance after letting it operate for a couple of minutes. If it looks O. K. , check balance. Walk to other side and move switch to test, wait for it to stabilize and adjust balance knob. Turn knob back to operate. Check that stripchart is marked properly for run date, instrument, stripchart settings, attenuation, *etc.*

### TSR and UV zero check

Mark time.

Check manifold on this side (RED). Start at the $NO_x$ and $O_3$ instrument end. (While you are at this end check zero air supply used for injections and be sure it is off.) Look for open fittings; missing caps or dangling sample lines. Feel heat tape; it should be warm. Look for condensation. Check zero air supply near stripchart for DP and HCHO. Move towards the other side of the bench. Check manifold fans to see that they are operating as you go around to the other side. Perform manifold check on this side walking to the end where the CARLEs are. Come back to the manifold fans. Check zero air supply. 100 lbs in and 60 lbs out. Check Tektronix terminal and clear screen by hitting page.

## GC Check

Check switch 6 on AUTO/MANUAL switch panel: is switch 6 on (Carles valve minders power)? Walk down towards Carles. On the way check the Varian stripchart. Are there injection peaks? H2O peaks? Tracer peaks? Is the sample pump on? Check that stripchart is marked properly for run date, instrument, stripchart settings, attenuation, *etc*. Check bucking current.

Are Carle valve minders in auto/repeat and sequencing? Do chromatograms look right? Air peaks? Look at example notebook if necessary. Are the GC sync? Do the chromatograms look right considering what was injected and the nature of today's run? Look at background chromatograms. Contamination? Ethylene? Was an autocal scheduled and were the chromatograms made? Peaks on scale for initial injection? Are they still on? Does it look like the baseline might drift off scale? Adjust with GC zero, not stripchart zero. Look at the service gas regulators. Do the readings match the numbers on the wall? Is the sample pump on? Is the 30 min RED/BLUE clock on and working? Is the flame lit? Reasonable attenuation getting? Are Sigma integrator reports being made?

Considering what was injected for the run:

- Target match condition? Are they matched?
- If difference, are the sides switching? Are both sets of chromatograms on scale (no peaks off scale)?
- If different amounts of same composition are ratios of peaks correct?
- Mark chromatograms with time and side. Try to mark time of sample injections.
- Try to mark when 30 min clock changes sides and whether B to R or R to B.
- Check that stripcharts are marked properly for run date, instrument, stripchart settings, attenuation, *etc*.

Check lab AC. Is it set at 72? Is fan in ON position (not AUTO)? When was the filter changed last? (It should be changed every three weeks.)

Enter PRINT PRO command if one is not printing already. Don't wait until later.

# Checklist for Leaving the Site Set Up for a Run

## Computer

Is the system up and ready?

- There has to be a day created on the disk for today in order for the system to run tomorrow.
- Create a day on the disk with tomorrow's date using the program "NEWDAY". If necessary, create one for today also.
- Create a command file for tomorrow using the Program "CMANDR". Once you are satisfied, store the command file by hitting "W". Now run the command file thru "DATRAN" and merge ("RMERGE") it into tomorrow's DATCOL-OPS file.
- Run DATCOL, wait 1 minute and you should see a "*", which will tell you that DATCOL is up; hit <RETURN> and you should get another *. If there was a run today, key in "BACK". This will print out the commands for the current day and tell you if the restart commands to vent the chambers (Set 1,2,3,4) at 1900 are still in there; otherwise the chambers won't vent!!! If there was not a run today, issue an immediate command IMM <return> and Set 1,2,3,4; to open the chamber doors.
- Are all front panel switches in auto not manual position; DVM on auto, rear, remote.
- Is the 4 minute clock switched to auto and not locked on one side?
- Check decwriter paper. Need at least 10 pages.

## Formaldehyde

- Run on water for 15 minutes by placing all three reagent tubes in water.
- Loosen all four tubes on parastatic pump.
- Shut off two switches on rear of instrument starting from the right as you face the switches. leave left most switch on. This supplies charging "juice" to the instrument batteries.
- Make sure there is enough TCM stock reagent prepared (without sulfite) so that the person making the run in the morning just has to add 0.25 g sulfite to 200 ml TMC.

## NOx and O3 Instruments

- Are the 3-way valves for the O3 and NOx meters plugged into the 4-minute power strip?
- Is there a good connection between the NOx and O3 meter intakes and the round Teflon filters?
- Are the front panel settings of the O3 and NOx meters correct?
    - The NOx meter should be in ambient mode. NO, NO2, and NOx should be set to 1 ppm full scale. The oxygen pressure should be set at 20, and the valve knob should be set to NO-NO2-NOx. Vacuum gauge on NOx pump should read 26" Hg.
    - The O3 meter should be set to 2 ppm and full scale. The ethylene pressure should be on 15. The time constant on the instrument should be set to 10 sec. The top of the + ethylene flow rotoball should be set at 30, and the mode selector should be set on ambient.
    - Strip Chart Recorder:
        - Pens on; on "record"
        - Chart "on"
        - Voltages 1, 1, 1/2 for NO, NO2, O3
        - Chart speed 3 cm/hr and "on"
    - Autocal Tank:
        - Tank should be turned on, 5 psi showing on low side of regulator, and on/off needle valve on regulator turned on.
        - Flow should have been previously adjusted so that meter will have enough sample when span tank is turned on in the morning (rotoball is positive showing excess flow when meter is sampling from this apparatus.

## TSR and UV Chart

- Have the TSR and UV pens been properly zeroed?

## Charts

- Check that sufficient paper remains Red line will appear on paper when the roll is ending.

- Record the date, type of injection, attenuation, chart speed and scale of each instrument on the charts.
- Check that pens are full of ink and pens down.
- Check that power to charts works from AC switch no. 16 on blue computer AC switch panel. Activate no. 16 to manual and observe deflection on charts, return these to "auto" position.

## Carle I

- Is the G.C. up and running?
    - Check pressure gauges on the wall behind the instrument H2 = 28.5 psi. He = 63 psi, air = 13.5 psi.
    - Is the flame lit? (check by placing mirror or chromed surface over the FID. It should fog H2 pressure to 35 psi, hit ignite button; you should see positive response on strip chart (strip chart has to be on) after 5 minutes. Return H2 to 28.5 psi. Watch the gauge go down and make sure it stabilizes at 28.5 psi.
    - Has the proper attenuation been dialed into Carle I? (X4 for mix, X8 for propylene and ethylene, everything else determined by the nature of the cal and the injection.
- Has the valve minder for Carle I been put on light no. 5 and a drum setting of 29?
    - To check this, activate switch no. 6 on the computer.
    - If the valveminder is not on light 5, switch the valveminder knob from "standby" to "sequence" at 10 second intervals until light no. 5 is on. While the valve minder know is in standby, rotate the timing drum until the face setting is 29. CHECK FLAME AGAIN. The valve minder knob should still be on standby at this time. Continue with Carle II and Carle III.

## Carle II and Carle III

- Is GC up and running?
    - Check pressure gauges on wall. Carle II, He = 38 psi, H2 = 27.5 psi, Air = 12.5 psi. Carle III, He = 64 psi, H2 = 28 psi, Air = 13.5 psi.
    - Check to see if flame is lit (place mirror over the FID).

  - Check for proper attenuation (normally X4).
- Have the valve minders for Carle II and III been placed on light 8 and a drum setting of 59?
  - To check this activate switch 6 on the computer.
  - If light 8 is not on, switch valve minder knob from "repeat" to "manual" and activate "event advance", toggle switch until light 8 is on. WAIT 10 SEC. BETWEEN EACH ADVANCE SWITCH. Make sure that you see light no. 7 before you advance to light no. 8. Set the drum at 59. CHECK FLAME AGAIN. Return to the computer blue switch panel and switch no. 6 to "auto". NOW GO BACK TO THE CARLES AND SWITCH CARLE I FROM STANDBY TO AUTO.
- ALSO TURN THE VALVE MINDER ON CARLE II AND III TO REPEAT. DO NOT LEAVE IN SINGLE OR OFF!!!

## Sigma 10 Integrator

- If we want to collect integrator data on the Sigma 10, Carle I, II, III must be linked to the Sigma by a "set up" procedure.

```
      SIGMA        (your key strokes)
     Response       SET UP KEY ENTER
EXAMPLE:
(1,2,4)    1 Enter
method?
1(2,4)       Enter
mode         Enter
Sample ID 1 Enter
           Carle (no. ) enter
Ptr        1 Enter
```

Note that: Carle 1 - Inst 1, Method 1., Carle II = Inst 2, Method 2, Carle III = Inst 4, Method 4. PE 900 = Inst 3, Method 41.

- If PE 900 is to be used, is it set up? Instrument 3 Method 4.
- Is there enough paper in the printer?
  - There are 199 sheets total, so if the printer has less than 20 sheets left, change the paper.
  - Void plotter unless you want to use it, it will otherwise use a lot of paper.

- Clear out old SIGMA files by using the following keystroke sequence: Shift*F6 enter 200 enter or Shift *F Enter Enter. Hit the "Stat" key after this is done. You should have at least 1000 free blocks.
- Turn the Tekronics terminal off (this is the second channel to the Sigma).

### Dew Point Meter

- Has the dew point meter been balanced and returned to operate? Set to "Test" and balance indicator to center of scale.
- Has the detector been cleaned within a week? Using isopropyl alcohol and Q-tip on mirror in detector in rear of instrument.
- Is the dew point meter chart been properly zeroed?
- Is the 3-way valve for the dew point meter plugged into the 4-minute power strip?

### ATC and Varian

Check standing current in morning and afternoon.

- Set the ATC and Varian injection clock right before injection.
- Is the ATC and Varian injection clock plugged into charts?
- Check to see if the ATC and Varian sampling 3-way valve is plugged into the 30 min red/blue clock and if the Teflon lines from the 3-way valve are attached to the red and blue sampling manifolds.
- Is the correct attenuation dialed into the Varian (atten x*)?
- Is the correct attenuation dialed into the ATC (X26)?

### CO Meter

- Is the sample line on the gas chambers?
- Turn off service air tank Back on in morning.
- Are front panel switches in correct position?

### Air Generators

Must have 100 psi on input gauge. and 60 psi on output gauge.

## General

(CHECK INJECTION TANK FLOW WITH BUBBLE METER EACH DAY AND SET TO 10 L/MIN)

- Check tanks for tomorrow's injections.
    - Go to the injection house and remove the line for the tank to be used from its control outlet.
    - Plug this line into the white power cord and read the tank flow on the mass flow meter.
    - If the flow rate is low or high adjust it with the low side pressure regulator valve. All tanks should have a flow of 10 l/min including NO.
    - Plug the tank line back into the control outlet for that tank.
- Check the following tanks in the service gas house: O3 ethylene NOx oxygen, Carle I He and H2, Carle II He and H2, CO3 and H2; Varian: ArCH4.
- Liquid Injections
    - Determine the number of ul that have to be injected from the computer listed table on the wall in back of the formaldehyde instrument. This table tells you the number of ul that you have to inject into the chamber to give 1 ppmC. This has been computed for three different temperatures 60 F, 70 F, and 80 F. Selected the number ul to be injected from the list which will approximate tomorrow's morning temperature. Clearly write down the number of ul to be injected on the run sheet.
    - Locate the liquids to be injected and set them out in the work space of the hood. Find the liquid injection apparatus and clean the needed syringes so that the operation will not have to spend time doing this tomorrow. Place these on a clean paper towel by the injection ports of the return manifold.
    - If you have to calculate the no. of ul to get 1 ppmC of a liquid into the chamber use the following formula:
- Has the run sheet been filled out?
- Have the charts been marked with day, month, year, instrument, chart speed, full scale chart voltage, and attenuation and range where applicable?
- Check for loose or missing caps on the manifolds.
- Check the chamber recirculation fans.
- Check all the red blue 3 way valves connected to the GCs to make sure they are plugged into the 30-min power outlet.
- Final check

- Check all auto/manual switches-computer and cal box-to make sure they are in auto position.
- Check DVM to make sure it is in remote not local mode. Especially 4 minute clock; it should be in auto.
- Check the red exhaust door on the chambers to see if it is the same as the blue exhaust door.
- Make sure all charts are on and plugged into "charts" strip.
- Check Carle I to be sure its valveminder is in auto and that Carle II and III valve minders are in repeat.
- Check high Conc. NOx calibration tank to be sure it is off.
- Check the Cal tank for the Carles to see that it is open.
- Check injection tanks to seer that they are open and that the flow is correct.
- Check the reagent levels for the HCHO instrument; also check the waste flask to see that it can't overfill.
- Shut off water to toilet.
- Make sure the chambers doors will open at 19:00, and vent by a Datcol Restart command, or by an immediate command to Datcol to set 1,2,3,4: before you leave the site.

## Early Morning Checkout

- Did the command file run? If not, see HELP LIST on end of rack over the DEC writer. Booting instructions are at other end of the rack over the disc.
- Is the DVM scanning? If not, issue an IMM to stop GASDVM; then, another IMM to start GASDVM. If DVM still is not scanning, switch from "Remote" to "Local". "Step" through to end of series (channel 60), return to "Remote" and issue an IMM to start GASDVM.
- Did the chambers vent? Check this by reading the $O_3$ strip chart–background should be almost completely free of $O_3$. If the chambers have not vented and enough time remains before sunrise–2.5 hours–manually vent chambers until just before sunrise. Close the chambers and then make all injections manually.
- Make CEA formaldehyde solutions.
- Read the run sheet and DEC printout of the day's command file to determine target concentrations.
- Find manual injection species and amounts and all apparatus necessary to make injections.
- Check chamber condensation and all vent doors (especially red exhaust door).
- Go to the injection house at the time of the injections to see if the lights confirm that the proper tanks are being injected. A list of tank concentrations, species, and switch numbers is on the end of the rack above the DEC writer.
- Check all charts.
    - Charts on at charts.
    - Pens down and full.
    - Charts fully labeled.
    - Sufficient chart paper for the day.
- Check manifolds to see that all caps are on and that each instrument is connected to both the red and blue manifolds.
- See that 4 minute computer clock is in AUTO and not locked manually to either side.
- Check status of SIGMA 10.
    - "/STAT"; all Carles and PE 900 (if used) should be set up with the corresponding methods.
        - ▹ Carle 1 Method 1
        - ▹ Carle 2 Method 2

        - ▷ Carle 3 Method 4
        - ▷ PE 900 Method 31
    - Check that sufficient paper remains for the day (about 75 sheets).
- Start CEA formaldehyde.
    - On sample line
    - Advanced past auto 0
    - All pump lines connected and useable and pulling solutions.
    - Sample pump on.
- Turn on air tank to the Beckman 6800 and turn on the instrument if it is to be used.
- Perform manual injections before 05:00 at the latest.
- Check standing current on the Varian: it should read about 600-9 x64 amps.
- Check injection concentrations and relate to target amounts by measuring peak heights and using the provided concentration conversion factors. See attached chromatograms.
    - $NO_x$: additive value from strip chart or from DVM printout.
    - Carle I,II,III: see attached chromatograms and respective values.
    - Adjust concentrations of $NO_x$ or HC species, if necessary, to achieve desired amounts.
- Change attenuation on the Carles after the auto cal; generally, attenuation should be x2 or x4.
- Issue a PRINT PROFILE of the DVM data.
- After successful injection turn off injection tanks and successful auto HC span turn off HCspan tank.

## Run Pack-Up Checklist

Before a run folder is taken to school, check to see if the following items are in it:

1. Carle I and II stripchart
2. Carle III stripchart
3. Sigma 10 printout
4. Varian stripchart
5. Dewpoint stripchart
6. Beckman stripchart
7. PE900 stripchart
8. DNPH integrator Printout and stripchart
9. TSR and UV stripchart
10. Formaldehyde stripchart
11. $NO_x$ and $O_3$ stripchart
12. Run Sheet
13. Instrument Checklist
14. Profile Printout
15. Copy of command file used
16. Copy of BAKTRN of the day's OPS file

If one of these is missing note reason on the instrument checklist.

# B

# HC Cal Sources Certification

# APPENDIX B.

## COMPARISON OF HYDROCARBON CALIBRATION SOURCES

```
                                        Last Update:  13-Jun-85

RTI TANKS             PRIMARY STANDARD #1 AND #2

                                 Species manuf.          Species manuf.
                                           conc.                   conc.
                               propylene 14.820        ethylene  20.000

                               27-Apr-78 14.580        27-Apr-78 19.400
                               22-May-78 14.820        25-May-78 19.200
                               23-May-78 14.340        10-Aug-78 19.800
                               08-Aug-78 14.940        05-May-80 16.800
                               14-May-80 14.790        19-Jul-81 20.000
                               03-Jan-84 14.400        29-May-84 19.000
ave USED                                 14.645                  19.480

regression estimate            02-Aug-84 14.449        02-Aug-84 19.304
------------------------------------------------------------------------
Calibration of Carles 1,2,3 with RTI tanks >> SIGMA 10 integrator ppmC/area

Assumption - these species are representative of average carbon response efficiency.
Did use May 5 1980 ethylene value.
Choice between regression value or average analysis value: used average.

                               UNC use:  14.645        UNC use:  19.480

Carle I               8/2/84 sigma 10  ppmc/area       sigma 10  ppmc/area
                                  44.6  0.328              56.3  0.346
                                  44.5  0.329              57.1  0.341
                                  44.5  0.329              57.2  0.341
                                  44.8  0.327

Ave                                     0.328                    0.343
allave                                                     0.335

                      8/1/84 sigma 10  ppmc/area
                                  44.8  0.327

                                        0.327
```

```
Carle II           8/2/84 sigma 10  ppmc/area      sigma 10  ppmc/area
                            19.1  0.767                24.7  0.789
                              19  0.771                24.4  0.798
                            19.2  0.763                24.8  0.785
                            19.6  0.747                24.8  0.785
                            19.2  0.763                24.5  0.795
                            19.1  0.767
                            18.9  0.775

Ave                               0.765                      0.791
allave                                                 0.778

                   8/1/84 sigma 10  ppmc/area      sigma 10  ppmc/area
                            17.4  0.842               25.31  0.770
                            19.2  0.763                24.7  0.789
                            19.3  0.759                24.7  0.789
                            20.5  0.714                25.2  0.773
                            19.3  0.759

ave                               0.767                      0.780
                                                       0.774

Carle III          8/2/84 sigma 10  ppmc/area
                            4.15  3.529
                            4.15  3.529
                            4.14  3.537
                            4.17  3.512
                            4.14  3.537

Ave                               3.529


                   8/1/84 sigma 10  ppmc/area
                            3.95  3.700
                            4.03  3.634
                            4.44  3.298

Ave                               3.547
```

```
------------------------------------------------------------------------------------------------------------------
Airco Tank - Determination of Concentration based on RTI tank - analyzed same day
Date                  toluene          ethylene      trans-2-butene   isopentane    propane         propylene
                        area     conc.   aroa             area          area            area          area
Carle I
8/2 - RTI ave ppmC/are 0.335
                       28.90                             21.30         28.00           22.00         24.80
                       29.90                             21.50         28.00           22.00         24.90
ave                    29.40      9.86                   21.40   7.18  28.00   9.39    22.00   7.38  24.85   8.34
8/1 - RTI ave ppmC/are 0.327
                       31.20                             22.70         29.70           23.60         26.20
                       31.50                             22.70         29.80           23.60         25.90
ave                    31.35     10.25                   22.70   7.42  29.75   9.73    23.60   7.71  26.05   8.52

Carle II
8/2 - RTI ave ppmC/are 0.778
                                         4.75   3.69                                    9.74   7.57  10.80   8.40
8/1 - RTI ave ppmC/are 0.774
                       16.20             5.08                                          10.60         11.60
                       14.50             4.03                                          10.30         11.40
                       14.20             4.75                                           9.66         10.90
                       14.70             4.81                                           9.64         11.00
ave                    14.90     11.53   4.87   3.77                                   10.05   7.78  11.23   8.68
Carle III
8/2 - RTI ave ppmC/are 3.529
                        3.22                              1.94          2.52
                        3.26                              1.96          2.55
ave                     3.24     11.43                    1.95   6.88   2.54   8.95
8/1 - RTI ave ppmC/are 3.547
                        3.30                              1.84          2.42
                        3.23                              1.90          2.47
                        3.24                              1.86          2.44
ave                     3.26     11.55                    1.87   6.62   2.44   8.67

THE AVERAGE -Airco tank          10.92          3.73             7.03          9.18            7.61          8.48
THE STD. DEV                      0.72          0.04             0.30          0.41            0.15          0.13
(these values are listed below - Airco Tank Final)
```

```
----------------------------------------------------------------------------------------------------------
CALIBRATION OF CARLES WITH AIRCO FOR ANALYSIS OF LOW AND HIGH MW HIGH CONC TANK - 7/18
"> <" indicates values not used in calculations
Date                  toluene           ethylene       trans-2-butene   isopentane    propane          propylene
                        area     conc.    area  conc.        area  conc.   area  conc.     area  conc.    area  conc.
                                10.92            3.73              7.03         9.18            7.61            8.48

Carle I
7/18- Cal with Airco standard
                                                             22.9       >  23.7 <NOT US    24.1             26.6
                        26.7                                 22.6          29.9            24.1             26.5
                        32.1                                 22.75         29.90           24.10            26.55
ave                     29.40                                 0.309         0.307           0.316            0.320
Cal today ppmC/area     0.372 <NOT USED
----------------------------------------------------------------------------------------------------------
ave Carle I ppmC/area   0.313

Carle II
7/18- Cal with Airco standard
                    >   18.2 <             5.55                                     >  15.1 <           11.8
                        15.4               5.15                                        11.5             11.9
                        15.2               5.53                                        10.5             11.6
                        15.8               6.04                                        11.8             11.9
ave                     15.47              5.57                                        11.27            11.80
Cal today ppmC/area      0.706             0.670                                        0.676            0.719
----------------------------------------------------------------------------------------------------------
ave Carle II ppmC/area  0.693

Carle III
7/18- Cal with Airco standard
                    >   4.17 < NOT USED                      1.92       >  3.94 <                  4.26 propane &
                        3.31                                 1.82          2.37                    4.27 propylene
                        3.26                                 1.82          2.41                    4.27
                        3.25                                 1.82          2.38                    4.27
                        3.27                                 1.97          2.40                    4.39
ave                     3.27                                 1.87          2.39                    4.292
Cal today ppmC/area     3.337 < NOT USED                     3.757         3.842                   3.750
```

```
------------------------------------------------------------------------------------------------------------------
ave Carle III ppmC/are 3.783

Date                  toluene          ethylene      trans-2-butene   isopentane    propane         propylene
                        area     conc.   area  conc.      area  conc.  area   conc.     area   conc.   area  conc.
                                 10.92          3.73            7.03          9.18             7.61          8.48

Carle I
8/14- Cal with Airco standard

                        26.3                              20.6          27.2            21.5          24.5
                        27.1                              20.9          27.4            21.3          23.8
ave                    26.70                             20.75         27.30           21.40         24.15
Cal today ppmC/area    0.409 < NOT USED                  0.339         0.336           0.356         0.351
------------------------------------------------------------------------------------------------------------------
ave Carle I ppmC/area  0.345


Carle II
8/14- Cal with Airco standard

                        13.5              4.7                                           9.58          10.5
                        13.9             4.62                                           9.31          10.3
ave                    13.70             4.66                                           9.45         10.40
Cal today ppmC/area    0.797            0.800                                          0.806         0.816
------------------------------------------------------------------------------------------------------------------
ave Carle II ppmC/area 0.805


Carle III
8/14- Cal with Airco standard

                        3.29                              1.95          2.57                   4.65 propane &
                        3.26                              1.97          2.57                   4.63
ave                     3.28                              1.96          2.57                   4.64
Cal today ppmC/area    3.336                             3.584         3.573                  3.469
------------------------------------------------------------------------------------------------------------------
ave Carle III ppmC/are 3.490
------------------------------------------------------------------------------------------------------------------
```

```
Liquid Injection Cals same day!
----------------------------------------------------------------------------------------------------
SIGMA 10 AREA CALS
Date                   toluene          m-xylene       o-xylene           pentane          2-me-pentane      di&tri-me-pentane
                          area    conc.   area   conc.      area   conc.   area    conc.       area   conc.   area   conc.
                                  2.99           2.98              2.66            2.99               3.16           5.98
Carle I
8/14- Cal with LIQUID standards

                          8.06            8.39              7.46
                          8.17            7.82              6.8            8.82            8.47             17
                          8.06            7.37              6.4            8.52            8.3              17.1
ave                       8.10            7.86              6.89           8.51            9.14             16.6
Cal today ppmC/area       0.369           0.379             0.387          8.62            8.64             16.90
                                                                           0.347           0.366            0.354
----------------------------------------------------------------------------------------------------
ave Carle I ppmC/area     0.367    aro    0.378     par     0.356 NOTE ARO CALS HIGHER THAN PAR
                                                   P/A=     0.94
Carle II
8/14- Cal with LIQUID standards

                          4.42            4.33              3.72
                          4.22            4.6               4.06
ave                       4.32            4.47              3.89
Cal today ppmC/area       0.692           0.667             0.685
----------------------------------------------------------------------------------------------------
ave Carle II ppmC/area 0.681


Carle III
8/14- Cal with LIQUID standards

                          0.989           0.917             0.797
                          0.983           0.931             0.800          0.812
                                          0.917             0.784          0.787
ave                       0.986           0.922             0.794          0.787
Cal today ppmC/area       3.030           3.230             3.355          0.795
                                                                           3.757
----------------------------------------------------------------------------------------------------
ave Carle III ppmC/are 3.343 NOTE DIFFERENCE BETWEEN AROS AND ALKANE
std dev                   0.2654
```

```
----------------------------------------------------------------------
PEAK HEIGHT CALS
Date                 toluene          m-xylene     o-xylene          pentane      2-me-pentane
                      ht in    conc.  ht in  conc.    ht in  conc. ht in  conc.    ht in  conc.
                                2.99         2.98             2.66         2.99            3.16

Carle I
8/14- Cal with LIQUID standards

                        6.8             3.4             2.4          8.4               6
                          7             3.4             2.4          8.4             5.8
                       6.86             3.3             2.4         8.36             5.8
ave                    6.89            3.37            2.40         8.39            5.87
Cal today ppmC/in     0.434           0.884           1.110        0.356           0.539
----------------------------------------------------------------------------------------------

Carle II
8/14- Cal with LIQUID standards

                        6.1             3.2             2.3
                        6.1             3.2             2.3
ave                    6.10            3.20            2.30
Cal today ppmC/in     0.490           0.930           1.158
----------------------------------------------------------------------

Carle III
8/14- Cal with LIQUID standards

                       13.2             7.3             5.2
                       13.2             7.3             5.2
ave                   13.20            7.30            5.20
Cal today ppmC/in     0.226           0.408           0.512
----------------------------------------------------------------------
```

```
------------------------------------------------------------------------------------------------------------
Low MW Hi Conc Tank - Determination of Concentration based on Airco Cals - analyzed same day
Date                   octane              ethylene/ethanbutanes-butenes   isopentane      propane           propylene
                         area      conc.    area              area            area             area              area
Carle I
7/18- AIRCO ave ppmC/a 0.313

                       288.60               35.50             274.90          56.50            66.00             66.90
                       300.10               38.10             277.10          56.80            67.00             67.30
ave                    294.35      92.08    36.80    11.51    276.00   86.34  56.65   17.72    66.50    20.80    67.10    20.99
Date                   pentane             2-me-1,3-butadiene
                         area      conc.    area
Carle I
7/18- AIRCO ave ppmC/a 0.313

                        63.80              132.40
                        63.80              133.90
ave                     63.80      19.96   133.15    41.65

Date                   octane              ethylene       ethane               propane/allenepropylene
                         area      conc.    area              area            area             area
Carle II
7/18- AIRCO ave ppmC/a 0.693

                       129.30               13.40              13.30          47.60            27.20
                                            13.30              14.40          47.10
ave                    129.30      89.56    13.35     9.25     13.85    9.59  47.35   32.80    27.20    18.84


Date                   octane              1-butene       n-butane             cis-2-butene  trans-butene    1,3-butadiene
                         area      conc.    area              area            area             area              area
Carle III
7/18- AIRCO ave ppmC/a 3.783

                        28.20                4.91               2.71           4.98             5.12              4.51
                        28.30                5.10               2.83           5.09             5.21              4.63
ave                     28.25     106.87     5.01    18.93      2.77   10.48   5.04   19.05     5.17    19.54     4.57    17.29
Date                   isopentane          pentane        propane/proplene/allene
                         area      conc.    area              area
Carle III
7/18- AIRCO ave ppmC/a 3.783

                         4.88                7.12              14.80
                         5.98                8.55              16.50
ave                      5.43      20.54     7.84    29.64     15.65   59.20
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 THE 7/13 HI TO LO CONC COMPARISON FOR LOMW  TANKS
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Low MW HI CONC Tank as source for cal for determination of LOMW LO CONC Cal Tank same day

Date                  octane          ethylene/ethanbutanes-butenes  isopentane    propane         propylene
7/13                    area     conc.  area             area          area            area          area
                                 96.17        18.84            85.29         17.72           20.80          20.99
Carle I
                      319.70                           261.30         59.00          53.70         62.00
                      299.70                           259.00         58.40          52.50         61.30
ave                   309.70                           260.15         58.70          53.10         61.65
Cal Today ppmC/area     0.31 <???                        0.33           0.38  .        0.39 <NOT US  0.34

Date                  pentane         2-me-1,3-butadiene
7/13                    area     conc.  area
                                 19.96        41.65
Carle I
                       65.40          138.30
                       65.00          136.50
ave                    65.20          137.40
Cal Today ppmC/area    0.306            0.303

Carle I ave ppmC/area  0.315

Date                  octane          ethylene      ethane           propane/allenepropylene
7/13                    area     conc.  area             area          area            area
                                 96.17         9.25             9.59         35.51           20.99
Carle II
                      148.30 <NOT USED 13.20            13.70         48.90          20.40
                      132.30          12.50             13.30         45.30 <NOT US  30.20
ave                   132.30          12.85             13.50         48.90          29.30
Cal Today ppmC/area    0.727           0.720             0.711         0.726          0.716

Carle II ave ppmC/area 0.720

Date                  octane          1-butene      n-butane         cis-2-butene  trans-butene    1,3-butadiene
7/13                    area     conc.  area             area          area            area          area
                                 96.17        18.93            10.48         19.05           19.54          17.29
Carle III
                       27.90            4.77             2.57          4.83            4.95          4.34
                       27.40            4.86             2.68          4.93            5.03          4.47
ave                    27.65            4.82             2.63          4.88            4.99          4.41
Cal Today ppmC/area     3.48 <NOT USED  3.93             3.99          3.90            3.92          3.92

Date                  isopentane      pentane       propane/proplene/allene
7/13                    area     conc.  area             area
                                 17.72        19.96            56.50
Carle III
                        4.43            4.78            14.40
                        4.51            4.95            14.60
ave                     4.47            4.87            14.50
Cal Today ppmC/area     3.96            4.10             3.90

Carle III ave ppmC/are  3.95
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Low MW Lo Conc Tank - Determination of Concentration based on HI conc Low MW Cals - analyzed same day

Date               octane        ethylene/ethanbutanes-butenes isopentane    propane    propylene
                     area   conc.  area           area            area          area         area
Carle I
7/13- LMWHI ave ppmC/a 0.315

                    19.62                        17.27            3.88          4.31         4.41
                    19.78                        17.28            3.83          4.07         4.85
ave                 19.70    6.21  0.00  0.00    17.28  5.44      3.86  1.21    4.19  1.32   4.63  1.46

Date               pentane       2-me-1,3-butadiene
                     area   conc.  area
Carle I
7/13- LMWHI ave ppmC/a 0.315

                     4.38          8.21
                     4.33
ave                  4.36    1.37  8.21  2.59

Date               octane        ethylene      ethane          propane/allenepropylene
                     area   conc.  area           area            area          area
Carle II
7/13- LMWHI ave ppmC/a 0.720

                                   1.87           1.19            3.45          2.67

ave                  0.00    0.00  1.87  1.35     1.19  0.86      3.45  2.48    2.67  1.92


Date               octane        1-butene      n-butane        cis-2-butene trans-butene  1,3-butadiene
                     area   conc.  area           area            area          area         area
Carle III
7/13- LMWHI ave ppmC/a 3.954

                     1.81          0.33           0.18                                       0.30
                     1.99          0.33           0.18            0.33          0.34         0.30
ave                  1.90    7.51  0.33  1.30     0.18  0.72      0.33  1.32    0.34  1.36   0.30  1.18

Date               isopentane    pentane       propane/proplene/allene
                     area   conc.  area           area
Carle III
7/13- LMWHI ave ppmC/a 3.954

                     0.31                         0.99
                     0.31                         0.99
ave                  0.31    1.22  0.00  0.00     0.99  3.91
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Low MW Tank as source for cal for determination of HMW Cal Tank same day

Date                  octane           ethylono/ethanbutanes-butones  isopentane    propane         propylene
5/30                    area     conc. area               area          area            area          area
                                 96.17         18.84            35.29         17.72           20.80         20.99
Carle I
                      329.00            56.70          281.40         58.30           70.30         68.40
                      336.10            56.50          280.50         57.70           70.20         68.20
ave                   332.55            56.60          200.95         58.00           70.25         68.30
Cal Today ppmC/area     0.29             0.33            0.30          0.31            0.30          0.31

Date                  pentane          2-me-1,3-butadiene
5/30                    area     conc. area
                                 19.96         41.65
Carle I
                       65.10           131.90
                       65.20           131.80
ave                    65.15           131.85
Cal Today ppmC/area    0.306            0.316

Carle I ave ppmC/area  0.307

Date                  octane           ethylene      ethane           propane/allenepropylene
5/30                    area     conc. area               area          area            area
                                 96.17          9.25             9.59         35.51           20.99
Carle II
                      129.70            12.80           13.40         48.10           28.80
                      129.70            12.60           13.20         48.70 <NOT US   26.50 <NOT USED
ave                   129.70            12.70           13.30         48.10           28.80
Cal Today ppmC/area    0.741            0.728           0.721         0.738           0.729

Carle II ave ppmC/area 0.732

Date                  octane           1-butene      n-butane         cis-2-butene  trans-butene    1,3-butadiene
5/30                    area     conc. area               area          area            area          area
                                 96.17         18.93            10.48         19.05           19.54         17.29
Carle III
                       28.30             4.63            2.54          4.69            4.75          4.30
                       28.30             4.67            2.56          4.72            4.80          4.30
ave                    28.30             4.65            2.55          4.71            4.78          4.30
Cal Today ppmC/area     3.40 <NOT USED   4.07            4.11          4.05            4.09          4.02
```

```
Date                    isopentane        pentane        propane/proplene/allene
5/30                       area     conc.   area               area
                                    17.72           19.96                 56.50
Carle III
                           4.30              4.71              13.90
                           4.32              4.72              13.90
ave                        4.31              4.72              13.90
Cal Today ppmC/area        4.11              4.23               4.06

Carle III ave ppmC/are   4.09

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High MW Tank - Determination of Concentration based on Airco Cals - analyzed same day

Date                       toluene         ethylbenzene  m-xylene          o-xylene      1-pentene
                             area     conc.   area  conc.      area  conc.   area  conc.     area  conc.
Carle I
7/18- AIRCO ave ppmC/a 0.313

                           60.50           63.50            61.90          60.80           49.60

ave                        60.50    18.93  63.50  19.86     61.90  19.36  60.80  19.02     49.60  15.52

Date                       toluene         ethylbenzene  m-xylene          o-xylene                     benzene
                             area     conc.   area               area          area                         area
Carle II
7/18- AIRCO ave ppmC/a 0.693

                           26.40           25.80            29.60          27.00                        24.00

ave                        26.40    18.29  25.80  17.87     29.60  20.50  27.00  18.70                  24.00  16.62

Date                       toluene         ethylbenzene  m-xylene          o-xylene      1-pentene      benzene
                             area     conc.   area  conc.      area  conc.   area  conc.     area  conc.  area
Carle III
7/18- AIRCO ave ppmC/a 3.783

                            6.12            6.42             6.80           6.37            7.21          5.74

ave                         6.12    23.15   6.42  24.29      6.80  25.72   6.37  24.10      7.21  27.27  5.74  21.71
                                                                                                  NOT USED
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Date                  isobutane         cyclohexane
                        area     conc.    area
Carle III
7/18- AIRCO ave ppmC/a 3.783

                        3.03              9.64

ave                     3.03     11.46    9.64  36.47

Date                   toluene          ethylbenzene  m-xylene           o-xylene         1-pentene
                        area     conc.    area  conc.      area   conc.   area   conc.      area   conc.
Carle I
8/14- AIRCO ave ppmC/a 0.345

                        54.84             59.31            57.65          55.37             44.68
                        55.94             61.65            60.26          58.22             44.88
ave                     55.39    19.14    60.48 20.89      58.96  20.37   56.80  19.62      44.78  15.47

Date                   toluene          ethylbenzene  m-xylene           o-xylene         acetylene         benzene
                        area     conc.    area             area           area               area             area
Carle II
8/14- AIRCO ave ppmC/a 0.805

                        24.42             25.19            30.66          25.87             20.61            23.00
                        24.63             25.77            31.12          26.31             21.70            23.10
ave                     24.53    19.74    25.48 20.51      30.89  24.86   26.09  21.00      21.16  17.03     23.05  18.55

Date                   toluene          ethylbenzene  m-xylene           o-xylene         1-pentene         benzene
                        area     conc.    area  conc.      area   conc.   area   conc.      area   conc.     area
Carle III
8/14- AIRCO ave ppmC/a 3.490

                        6.73              7.07             7.29           7.08              4.30             6.36
                        6.82              7.20             7.45           7.08              4.31             6.43
ave                     6.78     23.65    7.14  24.91      7.37   25.73   7.08   24.70      4.30   15.02     6.40   22.32
Date                  isobutane         cyclohexane
                        area     conc.    area
Carle III
8/14- AIRCO ave ppmC/a 3.490

                        3.37
                        3.38
ave                     3.37     11.77

Date                   toluene          ethylbenzene  m-xylene           o-xylene         1-pentene
                        area     conc.    area  conc.      area   conc.   area   conc.      area   conc.
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Carle I
8/14- LIQUID ave ppmC/ 0.367

                         54.84          59.31             57.65           55.37             44.68
                         55.94          61.65             60.26           58.22             44.88
ave                      55.39   20.32  60.48   22.19     58.96   21.63   56.80   20.84     44.78   16.43

Date                    toluene         ethylbenzene m-xylene           o-xylene        acetylene        benzene
                           area  conc.    area                area            area              area            area
Carle II
8/14- LIQUID ave ppmC/ 0.681

                         24.42          25.19             30.66           25.87             20.61           23.00
                         24.63          25.77             31.12           26.31             21.70           23.10
ave                      24.53   16.70  25.40   17.35     30.09   21.04   26.09   17.77     21.16   14.41   23.05   15.70

Date                    toluene         ethylbenzene m-xylene           o-xylene        1-pentene        benzene
                           area  conc.    area   conc.        area   conc.    area   conc.      area   conc.    area
Carle III
8/14- LIQUID ave ppmC/ 3.343

                          6.73            7.07              7.29            7.08              4.30            6.36
                          6.82            7.20              7.45            7.08              4.31            6.43
ave                       6.78   22.65    7.14   23.86      7.37   24.65    7.08   23.66      4.30   14.38    6.40   21.38

Date                    isobutane       cyclohexane
                           area  conc.    area
Carle III
8/14- LIQUID ave ppmC/ 3.343

                          3.37
                          3.38
ave                       3.37   11.27

Date                    toluene         m-xylene     o-xylene
                         ph x64  conc.   ph x64  conc.       ph in   conc.

Carle I
8/14-LIQ av ppmC/in x4 0.434              0.88                1.11

attn correction             16

                          2.95            1.55              1.27
                          3.00            1.60              1.30
ave                       2.98   20.65    1.58   22.28      1.29   22.81
```

| Date | toluene ph in | conc. | m-xylene ph in | conc. | o-xylene ph in | conc. |
|---|---|---|---|---|---|---|
| Carle II<br>8/14-LIQ av ppmC/in x4 | 0.490 | | 0.93 | | 1.16 | |
| attn correction | 16 | | | | | |
| | 2.47 | | 1.80 | | 1.22 | |
| | 2.50 | | | | 1.26 | |
| ave | 2.49 | 19.48 | 1.80 | 26.79 | 1.24 | 22.88 |

| Date | toluene ph in | conc. | m-xylene ph in | conc. | o-xylene ph in | conc. |
|---|---|---|---|---|---|---|
| Carle III<br>8/14-LIQ av ppmC/in x4 | 0.226 | | 0.41 | | 0.51 | |
| attn correction | 16 | | | | | |
| | 5.72 | | 3.72 | | 2.80 | |
| | 5.62 | | 3.80 | | 2.85 | |
| ave | 5.67 | 20.54 | 3.76 | 24.53 | 2.83 | 23.15 |

| Date | toluene area | conc. | ethylbenzene area | conc. | m-xylene area | conc. | o-xylene area | conc. | 1-pentene area | conc. | acetylene area | conc. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Carle I<br>5/30- LMWHC ave ppmC/a | 0.307 | | | | | | | | | | | |
| | 66.80 | | 66.50 | | 38.20 | | NA | | 48.60 | | 42.80 | |
| | 66.71 | | 67.70 | | 42.00 | | NA | | 48.60 | | 43.70 | |
| ave | 66.76 | 20.50 | 67.10 | 20.61 | 40.10 | 12.31 | NA | NA | 48.60 | 14.93 | 43.25 | 13.28 |

| Date | isobutane area | conc. |
|---|---|---|
| Carle I<br>5/30- LMWHC ave ppmC/a | 0.307 | |
| | 29.60 | |
| | 30.70 | |
| ave | 30.15 | 9.26 |

```
Date                  toluene          ethylbenzene  m-xylene         o-xylene      acetylene        benzene
                         area    conc.   area              area         area            area          area
Carle II
5/30- LMWHC ave ppmC/a 0.732

                        25.40           26.00             29.50         27.10          23.80         23.40
                        25.70           26.40             30.80         28.20          24.60         23.70
ave                     25.55    18.69  26.20  19.17      30.15 22.06   27.65 20.23    24.20  17.70   23.55  17.23

Date                  toluene          ethylbenzene  m-xylene         o-xylene     1-pentene         benzene
                         area    conc.   area conc.        area conc.   area  conc.     area  conc.   area
Carle III
5/30- LMWHC ave ppmC/a 4.094

                         5.83            6.08              6.24          5.97           3.63          5.48
                         5.80            6.17              6.32          6.05           3.61          5.47
ave                      5.82    23.81   6.13  25.07       6.28 25.71    6.01 24.60     3.62  14.82    5.48  22.41
Date                  isobutane        cyclohexane
                         area    conc.   area
Carle III
5/30- LMWHC ave ppmC/a 4.094

                         2.84            4.67
                         2.85            5.53
ave                      2.85    11.65   5.10  20.88


----------------------------------------------------------------------
                      Airco Tank
                                       OCS 112  UNC/
                      manuf. UNC- Dave UNC- Camanuf.
ethylene                 4.80     3.65    3.73  0.78
propylene                9.15     8.34    8.48  0.93
propane                  8.61     7.47    7.61  0.88
toluene                  9.94    10.72   10.92  1.10
trans-2-butene           6.92     6.91    7.03  1.02
isopentane               9.85     9.03    9.18  0.93

                                                0.94
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                           Low MW Tank HC
                         HIGH CONC                         OCS 109
                      manuf.  UNC-Dave U-Dave/Spread/     Spread             Carle I        Carle II          Carle ICarle III
                                       manuf. manuf.      Sheet              -------        ---------         -------
ethylene                10.0      9.32   0.93   0.92       9.25                               9.25
ethane                  10.0      9.84   0.98   0.96       9.59                               9.59  ______
propylene               21.9     20.70   0.95   0.96      20.99              20.99 _____     18.84       )
propane                 21.8     20.50   0.94   0.95      20.80              20.80 sum  )    32.80 sum   )   59.20     58.1
allene                  15.0     17.60   1.17   0.98      14.70  _____             _____)              ____)
1-butene                19.6     18.80   0.96   0.97      18.93        )                                   (   18.93     18.9
butane                  10.8     10.40   0.96   0.97      10.48        )                                   (   10.18     10.4
cis-2-butene            20.0     18.90   0.95   0.95      19.05  sum   )     86.34                    85.29    19.05     19.2
trans-2-butene          19.6     19.40   0.99   1.00      19.54        )                                   (   19.54     19.3
1,3-butadiene           20.0     17.20   0.86   0.86      17.29  _____ )                                   (   17.29     17.6
isopentane              18.1     17.40   0.96   0.98      17.72              17.72                             20.54     17.5
pentane                 20.0     19.70   0.99   1.00      19.96              19.96                             29.64     19.3
2-methyl-1,3-butadiene  17.1     41.40   2.42   2.44      41.65              41.65
octane                 104.2    104.00   1.00   0.92      96.17              92.08              89.56          106.87

                  ave                    0.97   0.96

                           Low MW Tank
                         HIGH CONC                 LOW CONC                 OCS 111
                      manuf.  UNC-Spd   UNC/      THC         UNC low/hi       UNC low/hi  low/hi/             Carle II ph der
                                       manuf. x 0.073         Dave           Spread        avg low/hi          5/30   7/13    avg
ethylene                10.0      9.25   0.92  0.675        0.634  0.069    0.629  0.068       0.99  -0.01   0.667  0.592  0.629
ethane                  10.0      9.59   0.96  0.700        0.644  0.067    0.628  0.065       0.95  -0.05   0.610  0.645  0.628
propylene               21.9     20.99   0.96  1.532        1.350  0.064    1.458  0.069       1.01   0.01                 0.000
propane                 21.8     20.80   0.95 ·1.519        1.310  0.063    1.320  0.063       0.93  -0.07                 0.000
allene                  15.0     14.70   0.98  1.073        1.240  0.084    1.148  0.078       1.14   0.14                 0.000
1-butene                19.6     18.93   0.97  1.382        1.300  0.069    1.305  0.069       1.01   0.01                 0.000
butane                  10.8     10.48   0.97  0.765        0.713  0.068    0.716  0.068       1.00    .00                 0.000
cis-2-butene            20.0     19.05   0.95  1.390        1.310  0.069    1.317  0.069       1.01   0.01                 0.000
trans-2-butene          19.6     19.54   1.00  1.426        1.350  0.069    1.356  0.069       1.01   0.01                 0.000
1,3-butadiene           20.0     17.29   0.86  1.262        1.180  0.068    1.184  0.068       1.00    .00                 0.000
isopentane              18.1     17.72   0.98  1.294        1.210  0.068    1.218  0.069       1.00    .00                 0.000
pentane                 20.0     19.96   1.00  1.457        1.340  0.067    1.372  0.069       1.00    .00                 0.000
2-methyl-1,3-butadiene  17.1     41.65   2.44  3.041        2.520  0.061    2.586  0.062       0.91  -0.09                 0.000
octane                 104.2     96.17   0.92  7.020        6.000  0.071    6.859  0.071       1.04   0.04                 0.000
                                                                                                        sd
not including 2-me-1,3-butadiene ave     0.96  0.073               0.068           0.069       1.00   0.05
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High MW Tank

| | | Carle I | | | | Carle II | | | | Carle III | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Sprd av | 5/30 | 7/18 | 8/14-T | 8/14-L | 5/30 | 7/18 | 8/14-T | 8/14-L | 5/30 | 7/18 | 8/14-T | 8/14-L |
| acetylene | 15.49 | 13.28 | | | | 17.704 | | | | | | | |
| isobutane | 11.08 | 9.26 | | | | | | | | 11.646 | 11.46 | 11.77 | 11.27 |
| 1-pentene | 15.22 | 14.93 | 15.52 | 15.47 | 16.43 | | | | | 14.819 | | 15.02 | 14.38 |
| benzene* | 19.49 | | | | | 17.228 | 16.62 | 18.55 | 15.70 | 22.413 | 21.71 | 22.32 | 21.38 |
| toluene* | 20.46 | 20.50 | 18.93 | 19.14 | 20.32 | 18.691 | 18.29 | 19.74 | 16.70 | 23.805 | 23.15 | 23.65 | 22.65 |
| ethylbenzene* | 21.38 | 20.61 | 19.86 | 20.89 | 22.19 | 19.167 | 17.87 | 20.51 | 17.35 | 25.074 | 24.29 | 24.91 | 23.86 |
| m-xylene* | 22.88 | 12.31 | 19.36 | 20.37 | 21.63 | 22.057 | 20.50 | 24.86 | 21.04 | 25.709 | 25.72 | 25.73 | 24.65 |
| o-xylene* | 21.29 | NA | 19.02 | 19.62 | 20.84 | 20.228 | 18.70 | 21.00 | 17.77 | 24.603 | 24.10 | 24.70 | 23.66 |

* AVE NOT USED

| | manuf. | Dave | ave/ manuf. | Meas. ave | Carle I | Carle I | Carle III |
|---|---|---|---|---|---|---|---|
| toluene | 21.10 | 20.40 | 0.96 | 20.22 | 20.65 | 19.48 | 20.54 |
| m-xylene | 22.30 | 23.50 | 1.05 | 23.41 | 22.20 | 26.79 | 24.53 |
| o-xylene | 22.40 | 22.50 | 1.02 | 22.95 | 22.81 | 22.08 | 23.15 |

*CARLE II M-XYLENE NOT USED

| | Car III ave | Meas. Car III | ave/Car III * ave res. |
|---|---|---|---|
| benzene* | 21.96 | | 20.00 |
| toluene* | 23.32 | 0.87 | |
| ethylbenzene* | 24.53 | | 22.34 |
| m-xylene* | 25.45 | 0.92 | |
| o-xylene* | 24.27 | 0.95 | |
| | ave res | 0.91 | |

High MW Tank

| | manuf. | UNC RTI-Dave | RTI-Dav manuf. | Sprd av manuf. | OCS 108 Sprd ave | Carle III Mo's 83 |
|---|---|---|---|---|---|---|
| acetylene | 14.60 | 12.90 | 0.88 | 1.06 | 15.49 | |
| isobutane | 12.00 | 11.30 | 0.94 | 0.92 | 11.08 | 12.20 |
| 1-pentene | 15.20 | 14.60 | 0.96 | 1.00 | 15.22 | 15.50 |
| benzene** | 20.00 | 20.00 | 1.00 | 1.00 | 20.00 | 22.70 |
| toluene* | 21.10 | 20.40 | 0.97 | 0.96 | 20.22 | 23.90 |
| ethylbenzene** | 23.80 | 22.50 | 0.95 | 0.94 | 22.34 | 24.30 |
| m-xylene* | 22.30 | 23.50 | 1.05 | 1.05 | 23.41 | 25.30 |
| o-xylene* | 22.40 | 22.50 | 1.00 | 1.02 | 22.95 | 23.50 |
| ave: | | | 0.97 | 0.99 | | |

```
                      Dimethylpentane   n-Octane      Ethylene          n-Butane      cis-butene
                        area      conc.   area  conc.       area  conc.   area  conc.      area  conc.
Carle I cal 5/30       79.10            117.80              8.50         26.30            23.90
ppmC/area =            81.80            130.50              8.52         26.40            24.10
               0.3071 -------           -------       ----------        -------       ---------
                       80.45      24.71 124.15  38.13       8.51   2.61  26.35   8.09     24.00   7.37

                      isopentane        2-me-1-butene propane           propylene
                        area      conc.   area  conc.       area  conc.   area  conc.
Carle I cal 5/30       41.40             39.90             19.40         18.20
ppmC/area =            41.60             40.40             19.70         18.40
               0.3071 -------           -------       ----------        -------
                       41.50      12.74  40.15  12.33      19.55   6.00  18.30   5.62


                                        n-Octane      Ethylene
                                          area  conc.       area  conc.
Carle II cal 5/30                        45.60              3.43
ppmC/area =                              48.80              3.43
               0.7316                   -------       ----------
                                         47.20  34.53       3.43   2.51

                                                      propane           propylene
                                                            area  conc.   area  conc.
Carle II cal 5/30                                           5.98          6.06
ppmC/area =                                                 6.00          6.02
               0.7316                                 ----------        -------
                                                            5.99   4.38   6.04   4.42


                                        n-Octane                        n-Butane      cis-butene
                                          area  conc.                     area  conc.      area  conc.
Carle III cal 5/30                       10.40                            1.90             1.78
ppmC/area =                              11.20                            1.89             1.77
               4.0938                   -------                         -------       ---------
                                         10.80  44.21                     1.90   7.76      1.78   7.27

                      isopentane        2-me-1-butene           propane/propylene
                        area      conc.   area  conc.             area  conc.
Carle III cal 5/30      3.03              3.21                    2.85
ppmC/area =             3.01              3.22                    2.83
               4.0938 -------           -------                 -------
                        3.02      12.36   3.22  13.16             2.84  11.63
```

```
                          manuf.    OCS #1   Car I  Car II   Car III     AVG  84/man.d rstd  84/OCS  d rstd
dimethylpentane          28.700    19.190  24.706                     24.706   0.86    0.56    1.29  -2.51
n-octane                 27.680    20.223  38.127  34.530    44.213  38.957   1.41   -3.75    1.93  -7.56 <not used
ethylene                  2.680     2.718   2.613   2.509             2.561   0.96   -0.19    0.94   0.22
n-butane                  8.000     7.979   8.092             7.758   7.925   0.99   -0.46    0.99  -0.18
cis-2-butene              6.800     8.000   7.370             7.267   7.318   1.08   -1.14    0.91   0.44
isopentane               19.500    12.971  12.745            12.363  12.554   0.64    2.27    0.97   0.02
2-me-1-butene            15.450    16.300  12.330            13.162  12.746   0.82.   0.85    0.78   1.49
propane                   6.060     6.119   6.004   4.382 <not used  6.004   0.99   -0.46    0.98  -0.08
propylene                 5.430     6.120   5.620   4.419 <not used  5.620   1.03   -0.81    0.92   0.42
propylene+propane         11.49    12.239  11.623            11.626  11.625   1.01   -0.63    0.95   0.17

                                                            ave         0.93             0.97
                                                            std dev     0.13             0.13

propylene- RTI
                N      X         Y     N*X     N*Y        EY       X2      Y2      XY             ploty
------------------------------------------------------------------------------------------       ------
                1      1     14.58       1   14.58 14.699452        1  212.57   14.58            14.58
                1     26     14.82      26   14.82 14.696710      676  219.63  385.32            14.82
                1     27     14.34      27   14.34 14.696601      729  205.63  387.18            14.34
                1    104     14.94     104   14.94 14.688156    10816  223.20  1553.7            14.94
                1    749     14.79     749   14.79 14.617417   561901  218.74  11077.            14.79
                1   2078      14.4    2078   14.40 14.471662    4E+06  207.36  29923.             14.4
------------------------------------------------------------------------------------------       ------
                6                     2985   87.87              5E+06  1287.1  43341.

                              YBAR:  14.645             sd:               SLOPE: -1.1E-04
                              XBAR:   497.5                               INTER: 14.69956
                                                                          R2:    0.138438

ethylene- RTI
                N      X         Y     N*X     N*Y        EY       X2      Y2      XY             ploty
------------------------------------------------------------------------------------------       ------
                1      1     19.40       1   19.40 19.558797        1  376.36    19.4             19.4
                1     29     19.20      29   19.20 19.555677      841  368.64   556.8             19.2
                1    106     19.80     106   19.80 19.547098    11236  392.04  2098.8             19.8
                0    740     16.00       0    0.00 19.476456        0       0       0               NA
                1   1180     20.00    1100   20.00 19.427431    1E+06     400   23600               20
                1   2225     19.00    2225   19.00 19.310995    5E+06     361   42275               19
------------------------------------------------------------------------------------------       ------
                5                     3541    97.4              6E+06  1898.0   68550

                              YBAR:   19.48             sd:               SLOPE: -1.1E-04
                              XBAR:   708.2                               INTER: 19.55890
                                                                          R2:    [illegible]
```

# C

# Official Calibration Sources

OFFICIAL CALIBRATION SOURCES 25-Sep-1985
Page 2

| ID NUM | DESC | SDATE | SER NUM |  | STATED CONC | ACTUAL CONC |
|---|---|---|---|---|---|---|
| 23 | TOLUENEINJ | 18-Aug-1983 | NA | TOLUENE | 0.795 | 0.795 |
| 24 | TOLUENEINJ | 26-Aug-1983 | NA | TOLUENE | 0.788 | 0.788 |
| 25 |  |  |  |  | 0.000 | 0.000 |
| 26 |  |  |  |  | [illegible] | 0.000 |
| 27 | TOLUENEINJ | 22-Aug-1983 | NA | TOLUENE | 0.[illegible] | [illegible] |
| 28 | MXYLENEINJ | 22-Aug-1983 | NA | M-XYLENE | 0.534 | 0.58[illegible] |
| 29 | TOLUENEINJ | 6-Oct-1983 | NA | TOLUENE | 0.381 | 0.381 |
| 30 | TOLUENEINJ | 6-Oct-1983 | NA | TOLUENE | 0.381 | 0.381 |
| 31 | 124TMBINJB | 6-Oct-1983 | NA | 1,2,4-TRIMETHYLBENZENE | 0.233 | 0.233 |
| 32 | 124TMBINJR | 6-Oct-1983 | NA | 1,2,4-TRIMETHYLBENZENE | 0.233 | 0.233 |
| 33 | MXYLENEINJ | 6-Oct-1983 | NA | M-XYLENE | 0.180 | 0.180 |
| 34 | MXYLENEINJ | 6-Oct-1983 | NA | M-XYLENE | 0.180 | 0.180 |
| 35 | OXYLENEINJ | 6-Oct-1983 | NA | O-XYLENE | 0.111 | 0.111 |
| 36 | OXYLENEINJ | 6-Oct-1983 | NA | O-XYLENE | 0.111 | 0.111 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | 2-METHYLPENTANE | 1.000 | 1.000 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | 2,3-DIMETHYLPENTANE | 1.000 | 1.000 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | METHYLCYCLOHEXANE | 1.000 | 1.000 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | TOLUENE | 1.000 | 1.000 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | ETHYLBENZENE | 1.000 | 1.000 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | M-XYLENE | 1.000 | 1.000 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | N-PROPYLBENZENE | 1.000 | 1.000 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | 2,2,4-TRIMETHYLPENTANE | 1.000 | 1.000 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | TERT-BUTYLBENZENE | 1.000 | 1.000 |
| 37 | PE900CLMX4 | 23-Jul-1983 | NA | 1,3,5-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 38 | TOLUENEINJ | 25-Jul-1983 | NA | TOLUENE | 0.601 | 0.601 |
| 39 | ISOPENTINJ | 25-Jul-1983 | NA | ISOPENTANE | 0.166 | 0.166 |
| 40 | 124TMBINJ | 25-Jul-1983 | NA | 1,2,4-TRIMETHYLBENZENE | 0.369 | 0.369 |
| 41 | TOLUENEINJ | 25-Jul-1983 | NA | TOLUENE | 0.601 | 0.601 |
| 42 | ISOPENTINJ | 25-Jul-1983 | NA | ISOPENTANE | 0.166 | 0.166 |
| 43 | 124TMBINJ | 25-Jul-1983 | NA | 1,2,4-TRIMETHYLBENZENE | 0.369 | 0.369 |
| 44 | TOLUENEINJ | 8-Aug-1983 | NA | TOLUENE | 9.125 | 9.125 |
| 45 | OXYLENEINJ | 8-Aug-1983 | NA | O-XYLENE | 6.083 | 6.083 |
| 46 | METOLINJ | 9-Aug-1983 | NA | M-ETHYLTOLUENE | 4.000 | 4.000 |
| 47 | 224TMPINJ | 19-Aug-1983 | NA | 2,2,4-TRIMETHYLPENTANE | 4.053 | 4.053 |
| 48 | ISOPENINJ | 19-Aug-1983 | NA | ISOPENTANE | 4.059 | 4.059 |
| 49 | OXYLENEINJ | 1-Aug-1983 | NA | O-XYLENE | 2.699 | 2.699 |
| 50 | TOLUENEINJ | 1-Aug-1983 | NA | TOLUENE | 4.553 | 4.529 |
| 51 | DETHKETINJ | 20-Jun-1983 | NA | 3-PENTANONE | 1.010 | 1.010 |
| 52 | DETHKETINJ | 20-Jun-1983 | NA | 3-PENTANONE | 1.010 | 1.010 |
| 53 | PE900CLMXS | 9-Sep-1983 |  | BENZENE | 1.000 | 1.000 |
| 53 | PE900CLMXS | 9-Sep-1983 |  | P-XYLENE | 1.000 | 1.000 |
| 53 | PE900CLMXS | 9-Sep-1983 |  | O-XYLENE | 1.000 | 1.000 |
| 53 | PE900CLMXS | 9-Sep-1983 |  | 1,2,4-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 53 | PE900CLMXS | 9-Sep-1983 |  | SEC-BUTYLBENZENE | 1.000 | 1.000 |
| 53 | PE900CLMXS | 9-Sep-1983 |  | M-ETHYLTOLUENE | 1.000 | 1.000 |

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| ID NUM | DESC | SDATE | SER NUM | | STATED CONC | ACTUAL CONC |
|---|---|---|---|---|---|---|
| 53 | PE900CLMXS | 9-Sep-1983 | | ISOPROPYLBENZENE | 1.000 | 1.000 |
| 53 | PE900CLMXS | 9-Sep-1983 | | 1,2,3-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 53 | PE900CLMXS | 9-Sep-1983 | | BUTYLBENZENE | 1.000 | 1.000 |
| 54 | NEW83COCH4 | 30-Sep-1983 | | METHANE | 4.934 | 4.934 |
| 54 | NEW83COCH4 | 30-Sep-1983 | | CO | 5.114 | 5.114 |
| 55 | PE900CLMXS | 3-Oct-1983 | | BENZENE | 1.000 | 1.000 |
| 55 | PE900CLMXS | 3-Oct-1983 | | P-XYLENE | 1.000 | 1.000 |
| 55 | PE900CLMXS | 3-Oct-1983 | | O-XYLENE | 1.000 | 1.000 |
| 55 | PE900CLMXS | 3-Oct-1983 | | 1,2,4-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 55 | PE900CLMXS | 3-Oct-1983 | | SEC-BUTYLBENZENE | 1.000 | 1.000 |
| 55 | PE900CLMXS | 3-Oct-1983 | | M-ETHYLTOLUENE | 1.000 | 1.000 |
| 55 | PE900CLMXS | 3-Oct-1983 | | ISOPROPYLBENZENE | 1.000 | 1.000 |
| 55 | PE900CLMXS | 3-Oct-1983 | | 1,2,3-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 55 | PE900CLMXS | 3-Oct-1983 | | BUTYLBENZENE | 1.000 | 1.000 |
| 56 | PE900CLMXS | 4-Sep-1983 | | BENZENE | 1.000 | 1.000 |
| 56 | PE900CLMXS | 4-Sep-1983 | | P-XYLENE | 1.000 | 1.000 |
| 56 | PE900CLMXS | 4-Sep-1983 | | O-XYLENE | 1.000 | 1.000 |
| 56 | PE900CLMXS | 4-Sep-1983 | | 1,2,4-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 56 | PE900CLMXS | 4-Sep-1983 | | SEC-BUTYLBENZENE | 1.000 | 1.000 |
| 56 | PE900CLMXS | 4-Sep-1983 | | M-ETHYLTOLUENE | 1.000 | 1.000 |
| 56 | PE900CLMXS | 4-Sep-1983 | | ISOPROPYLBENZENE | 1.000 | 1.000 |
| 56 | PE900CLMXS | 4-Sep-1983 | | 1,2,3-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 56 | PE900CLMXS | 4-Sep-1983 | | BUTYLBENZENE | 1.000 | 1.000 |
| 57 | PE900CLMXS | 24-Jun-1983 | | BENZENE | 1.000 | 1.000 |
| 57 | PE900CLMXS | 24-Jun-1983 | | P-XYLENE | 1.000 | 1.000 |
| 57 | PE900CLMXS | 24-Jun-1983 | | O-XYLENE | 1.000 | 1.000 |
| 57 | PE900CLMXS | 24-Jun-1983 | | 1,2,4-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 57 | PE900CLMXS | 24-Jun-1983 | | SEC-BUTYLBENZENE | 1.000 | 1.000 |
| 57 | PE900CLMXS | 24-Jun-1983 | | M-ETHYLTOLUENE | 1.000 | 1.000 |
| 57 | PE900CLMXS | 24-Jun-1983 | | ISOPROPYLBENZENE | 1.000 | 1.000 |
| 57 | PE900CLMXS | 24-Jun-1983 | | 1,2,3-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 57 | PE90CLMXS | 24-Jun-1983 | | BUTYLBENZENE | 1.000 | 1.000 |
| 58 | PE900CLMXS | 30-Jun-1983 | | BENZENE | 1.000 | 1.000 |
| 58 | PE900CLMXS | 30-Jun-1983 | | P-XYLENE | 1.000 | 1.000 |
| 58 | PE900CLMXS | 30-Jun-1983 | | O-XYLENE | 1.000 | 1.000 |
| 58 | PE900CLMXS | 30-Jun-1983 | | 1,2,4-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 58 | PE900CLMXS | 30-Jun-1983 | | SEC-BUTYLBENZENE | 1.000 | 1.000 |
| 58 | PE900CLMXS | 30-Jun-1983 | | M-ETHYLTOLUENE | 1.000 | 1.000 |
| 58 | PE900CLMXS | 30-Jun-1983 | | ISOPROPYLBENZENE | 1.000 | 1.000 |
| 58 | PE900CLMXS | 30-Jun-1983 | | 1,2,3-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 58 | PE900CLMXS | 30-Jun-1983 | | BUTYLBENZENE | 1.000 | 1.000 |
| 59 | PE900CLMX4 | 3-Jun-1983 | | 2-METHYLPENTANE | 1.000 | 1.000 |
| 59 | PE900CLMXS | 3-Jun-1983 | | 2,3-DIMETHYLPENTANE | 1.000 | 1.000 |
| 59 | PE900CLMXS | 3-Jun-1983 | | METHYLCYCLOHEXANE | 1.000 | 1.000 |

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                   OFFICIAL CALIBRATION SOURCES                   25-Sep-1985
                                                                  Page 4

ID                                    SER
NUM    DESC         SDATE             NUM                                    STATED   ACTUAL
                                                                             CONC     CONC
 59  PE900CLMXS   3-Jun-1983                 TOLUENE                       1.000    1.000
 59  PE900CLMXS   3-Jun-1983                 ETHYLBENZENE                  1.000    1.000
 59  PE900CLMXS   3-Jun-1983                 M-XYLENE                      1.000    1.000
 59  PE900CLMXS   3-Jun-1983                 N-PROPYLBENZENE               1.000    1.000
 59  PE900CLMXS   3-Jun-1983                 2,2,4-TRIMETHYLPENTA          1.000    1.000
                                             NE
 59  PE900CLMXS   3-Jun-1983                 TERT-BUTYLBENZENE             1.000    1.000
 59  PE900CLMXS   3-Jun-1983                 1,3,5-TRIMETHYLBENZE          1.000    1.000
                                             NE
 60  PE900CLMXS   6-Jul-1983   NA                  BENZENE                       1.000    1.000
 60  PE900CLMXS   6-Jul-1983   NA                  P-XYLENE                      1.000    1.000
 60  PE900CLMXS   6-Jul-1983   NA                  O-XYLENE                      1.000    1.000
 60  PE900CLMXS   6-Jul-1983   NA                  1,2,4-TRIMETHYLBENZE          1.000    1.000
                                             NE
 60  PE900CLMXS   6-Jul-1983   NA                  SEC-BUTYLBENZENE              1.000    1.000
 60  PE900CLMXS   6-Jul-1983   NA                  M-ETHYLTOLUENE                1.000    1.000
 60  PE900CLMXS   6-Jul-1983   NA                  ISOPROPYLBENZENE              1.000    1.000
 60  PE900CLMXS   6-Jul-1983   NA                  1,2,3-TRIMETHYLBENZE          1.000    1.000
                                             NE
 60  PE900CLMXS   6-Jul-1983   NA                  BUTYLBENZENE                  1.000    1.000
 61  PE900CLMX5  18-Jul-1983   NA            BENZENE                       1.000    1.000
 61  PE900CLMX5  18-Jul-1983   NA            P-XYLENE                      1.000    1.000
 61  PE900CLMX5  18-Jul-1983   NA            O-XYLENE                      1.000    1.000
 61  PE900CLMX5  18-Jul-1983   NA            1,2,4-TRIMETHYLBENZE          1.000    1.000
                                             NE
 61  PE900CLMX5  18-Jul-1983   NA            SEC-BUTYLBENZENE              1.000    1.000
 61  PE900CLMX5  18-Jul-1983   NA            M-ETHYLTOLUENE                1.000    1.000
 61  PE900CLMX5  18-Jul-1983   NA            ISOPROPYLBENZENE              1.000    1.000
 61  PE900CLMX5  18-Jul-1983   NA            1,2,3-TRIMETHYLBENZE          1.000    1.000
                                             NE
 61  PE900CLMX5  18-Jul-1983   NA            BUTYLBENZENE                  1.000    1.000
 62  PE900CLMX4  18-Jul-1983                 2-METHYLPENTANE               1.000    1.000
 62  PE900CLMX4  18-Jul-1983                 2,3-DIMETHYLPENTANE           1.000    1.000
 62  PE900CLMX4  18-Jul-1983                 METHYLCYCLOHEXANE             1.000    1.000
 62  PE900CLMX4  18-Jul-1983                 TOLUENE                       1.000    1.000
 62  PE900CLMX4  18-Jul-1983                 ETHYLBENZENE                  1.000    1.000
 62  PE900CLMX4  18-Jul-1983                 M-XYLENE                      1.000    1.000
 62  PE900CLMX4  18-Jul-1983                 N-PROPYLBENZENE               1.000    1.000
 62  PE900CLMX4  18-Jul-1983                 2,2,4-TRIMETHYLPENTA          1.000    1.000
                                             NE
 62  PE900CLMX4  18-Jul-1983                 TERT-BUTYLBENZENE             1.000    1.000
 62  PE900CLMX4  18-Jul-1983                 1,3,5-TRIMETHYLBENZE          1.000    1.000
                                             NE
 63  PE900CLMX5  23-Jul-1983                 BENZENE                       1.000    1.000
 63  PE900CLMX5  23-Jul-1983                 P-XYLENE                      1.000    1.000
 63  PE900CLMX5  23-Jul-1983                 O-XYLENE                      1.000    1.000
 63  PE900CLMX5  23-Jul-1983                 1,2,4-TRIMETHYLBENZE          1.000    1.000
                                             NE
 63  PE900CLMX5  23-Jul-1983                 SEC-BUTYLBENZENE              1.000    1.000
 63  PE900CLMX5  23-Jul-1983                 M-ETHYLTOLUENE                1.000    1.000
 63  PE900CLMX5  23-Jul-1983                 ISOPROPYLBENZENE              1.000    1.000
 63  PE900CLMX5  23-Jul-1983                 1,2,3-TRIMETHYLBENZE          1.000    1.000
                                             NE
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| ID NUM | DESC | SDATE | SER NUM | | STATED CONC | ACTUAL CONC |
|---|---|---|---|---|---|---|
| 63 | PE900CLMX5 | 23-Jul-1983 | | BUTYLBENZENE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | 2-METHYLPENTANE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | 2,3-DIMETHYLPENTANE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | METHYLCYCLOHEXANE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | TOLUENE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | ETHYLBENZENE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | M-XYLENE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | N-PROPYLBENZENE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | 2,2,4-TRIMETHYLPENTANE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | TERT-BUTYLBENZENE | 1.000 | 1.000 |
| 64 | PE900CLMX4 | 23-Jul-1983 | | 1,3,5-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 65 | PE900CLMX5 | 2-Aug-1983 | | BENZENE | 1.000 | 1.000 |
| 65 | PE900CLMX5 | 2-Aug-1983 | | P-XYLENE | 1.000 | 1.000 |
| 65 | PE900CLMX5 | 2-Aug-1983 | | O-XYLENE | 1.000 | 1.000 |
| 65 | PE900CLMX5 | 2-Aug-1983 | | 1,2,4-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 65 | PE900CLMX5 | 2-Aug-1983 | | SEC-BUTYLBENZENE | 1.000 | 1.000 |
| 65 | PE900CLMX5 | 2-Aug-1983 | | M-ETHYLTOLUENE | 1.000 | 1.000 |
| 65 | PE900CLMX5 | 2-Aug-1983 | | ISOPROPYLBENZENE | 1.000 | 1.000 |
| 65 | PE900CLMX5 | 2-Aug-1983 | | 1,2,3-TRIMETHYLBENZENE | 1.000 | 1.000 |
| 65 | PE900CLMX5 | 2-Aug-1983 | | BUTYLBENZENE | 1.000 | 1.000 |
| 66 | HCOHINJ | 6-Jun-1983 | | FORMALDEHYDE | 1.072 | 1.072 |
| 67 | HCOHINJ | 15-Jun-1983 | | FORMALDEHYDE | 1.000 | 1.000 |
| 68 | HCOHINJ | 24-Nov-1983 | | FORMALDEHYDE | 1.024 | 1.024 |
| 69 | HCOHINJ | 18-Jun-1983 | | FORMALDEHYDE | 1.041 | 1.041 |
| 70 | HCOHINJ | 12-Jul-1983 | | FORMALDEHYDE | 1.029 | 1.029 |
| 71 | HCOHINJ | 12-Aug-1983 | | FORMALDEHYDE | 1.032 | 0.000 |
| 72 | HCOHINJ | 23-Jul-1983 | | FORMALDEHYDE | 1.047 | 1.047 |
| 73 | HCOHINJ | 29-Jul-1983 | | FORMALDEHYDE | 1.026 | 1.026 |
| 74 | HCOHINJ | 13-Aug-1983 | | FORMALDEHYDE | 1.016 | 1.016 |
| 75 | HCOHINJ | 19-Sep-1983 | | FORMALDEHYDE | 1.026 | 1.026 |
| 76 | NO2ASPAN | 10-Jun-1983 | | PAN | 0.244 | 0.244 |
| 77 | NO2ASPAN | 18-Jun-1983 | | PAN | 0.152 | 0.152 |
| 78 | NO2ASPAN | 13-Jul-1983 | | PAN | 0.037 | 0.037 |
| 79 | NO2ASPAN | 17-Jul-1983 | | PAN | 0.071 | 0.071 |
| 80 | no2aspan | 18-Jul-1983 | | PAN | 0.055 | 0.055 |
| 81 | no2aspan | 20-Jul-1983 | | PAN | 0.081 | 0.081 |
| 82 | no2aspan | 21-Jul-1983 | | PAN | 0.061 | 0.061 |
| 83 | no2aspan | 26-Jul-1983 | | PAN | 0.025 | 0.025 |
| 84 | no2aspan | 29-Jul-1983 | | PAN | 0.074 | 0.074 |
| 85 | no2aspan | 31-Jul-1983 | | PAN | 0.059 | 0.059 |
| 86 | no2aspan | 4-Aug-1983 | | PAN | 0.036 | 0.036 |
| 87 | no2aspan | 13-Aug-1983 | | PAN | 0.074 | 0.074 |
| 88 | no2aspan | 5-Sep-1983 | | PAN | 0.105 | 0.105 |
| 89 | no2aspan | 7-Sep-1983 | | PAN | 0.096 | 0.096 |
| 90 | no2aspan | 18-Sep-1983 | | PAN | 0.114 | 0.114 |
| 91 | no2aspan | 23-Sep-1983 | | PAN | 0.100 | 0.100 |
| 92 | no2aspan | 2-Oct-1983 | | PAN | 0.200 | 0.200 |
| 93 | NO2ASPAN | 14-Oct-1983 | | PAN | 0.110 | 0.110 |
| 94 | NO46PPMCAL | 22-Jun-1934 | SX13759 | NO. | 46.000 | 52.600 |

# OFFICIAL CALIBRATION SOURCES

| ID NUM | DESC | SDATE | SER NUM | | STATED CONC | ACTUAL CONC |
|---|---|---|---|---|---|---|
| 95 | MXYLENEINJ | 25-Jun-1984 | | M-XYLENE | 3.000 | 2.963 |
| 96 | TOLUENEINJ | 25-Jun-1984 | | TOLUENE | 6.000 | 5.895 |
| 97 | TOLUENE | 27-Jun-1984 | | TOLUENE | 5.000 | 4.909 |
| 98 | M-XYLENE | 26-Jun-1984 | | M-XYLENE | 3.000 | 2.973 |
| 99 | O-XYLENE | 26-Jun-1984 | | O-XYLENE | 3.000 | 2.653 |
| 100 | TOLUENE | 19-Jun-1984 | | TOLUENE | 4.000 | 3.929 |
| 101 | M-XYLENE | 19-Jun-1984 | | M-XYLENE | 3.000 | 2.967 |
| 102 | FORMALDEHY | 10-Jul-1984 | | FORMALDEHYDE | 0.500 | 0.542 |
| 103 | FORMALDEHY | 10-Jul-1984 | | FORMALDEHYDE | 1.060 | 1.035 |
| 104 | HCHOINJB | 11-Jul-1984 | NA | FORMALDEHYDE | 1.000 | 0.945 |
| 105 | HCHOINJR | 11-Jul-1984 | NA | FORMALDEHYDE | 1.000 | 0.946 |
| 106 | HCHOINJRAF | 27-Jul-1984 | NA | FORMALDEHYDE | 1.000 | 0.946 |
| 107 | HCHOINJRMO | 27-Jul-1984 | NA | FORMALDEHYDE | 0.200 | 0.189 |
| 108 | HIMWHICONC | | | ACETYLENE | 14.600 | 15.490 |
| 108 | HIMWHICONC | | | ISOBUTANE | 12.000 | 11.080 |
| 108 | HIMWHICONC | | | 1-PENTENE | 15.175 | 15.200 |
| 108 | HIMWHICONC | | | BENZENE | 19.956 | 19.910 |
| 108 | HIMWHICONC | | | TOLUENE | 21.056 | 20.300 |
| 108 | HIMWHICONC | | | ETHYLBENZENE | 23.784 | 22.250 |
| 108 | HIMWHICONC | | | M-XYLENE | 22.272 | 23.590 |
| 108 | HIMWHICONC | | | O-XYLENE | 22.432 | 22.950 |
| 109 | LOMWHICONC | | | ETHYLENE | 10.064 | 9.250 |
| 109 | LOMWHICONC | | | ETHANE | 10.000 | 9.590 |
| 109 | LOMWHICONC | | | PROPYLENE | 21.996 | 20.990 |
| 109 | LOMWHICONC | | | PROPANE | 21.894 | 20.300 |
| 109 | LOMWHICONC | | | PROPADIENE | 15.000 | 14.700 |
| 109 | LOMWHICONC | | | 1-BUTENE | 19.600 | 18.930 |
| 109 | LOMWHICONC | | | N-BUTANE | 10.300 | 10.480 |
| [illegible] | LOMWHICONC | | | 1,3-BUTADIENE | 20.000 | 17.290 |
| 109 | LOMWHICONC | | | TRANS-2-BUTENE | 20.000 | 19.540 |
| 109 | LOMWHICONC | | | CIS-2-BUTENE | 20.000 | 19.050 |
| 109 | LOMWHICONC | | | ISOPENTANE | 18.135 | 17.7[illegible] |
| 109 | LOMWHICONC | | | N-PENTANE | 19.956 | 19.960 |
| 109 | LOMWHICONC | | | N-OCTANE | ****** | 96.170 |
| 109 | LOMWHICONC | | | 2-METHYL-1,3-BUTADIENE | 17.055 | 41.650 |
| 110 | SCOTT84 | | | ETHYLENE | 0.600 | 0.711 |
| 110 | SCOTT84 | | | PROPYLENE | 0.900 | 1.128 |
| 110 | SCOTT84 | | | PROPANE | 0.900 | 0.972 |
| 110 | SCOTT84 | | | CIS-2-BUTENE | 1.000 | 1.110 |
| 110 | SCOTT84 | | | ISOPENTANE | 1.250 | 1.145 |
| 110 | SCOTT84 | | | N-PENTANE | 1.250 | 1.347 |
| 110 | SCOTT84 | | | TOLUENE | 2.800 | 3.250 |
| 110 | SCOTT84 | | | 2-METHYL-2-BUTENE | 1.250 | 1.390 |
| 111 | LOMWLOCONC | | | ETHYLENE | 0.000 | 0.629 |
| 111 | LOMWLOCONC | | | ETHANE | 0.000 | 0.628 |
| 111 | LOMWLOCONC | | | PROPYLENE | 0.000 | 1.458 |
| 111 | LOMWLOCONC | | | PROPANE | 0.000 | 1.320 |
| 111 | LOMWLOCONC | | | PROPADIENE | 0.000 | 1.148 |
| 111 | LOMWLOCONC | | | 1-BUTENE | 0.000 | 1.305 |
| 111 | LOMWLOCONC | | | N-BUTANE | 0.000 | 0.716 |
| 111 | LOMWLOCONC | | | 1,3-BUTADIENE | 0.000 | 1.184 |
| 111 | LOMWLOCONC | | | TRANS-2-BUTENE | 0.000 | 1.356 |

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# OFFICIAL CALIBRATION SOURCES

| ID NUM | DESC | SDATE | SER NUM | | STATED CONC | ACTUAL CONC |
|---|---|---|---|---|---|---|
| 111 | LOMWLOCONC | | | CIS-2-BUTENE | 0.000 | 1.317 |
| 111 | LOMWLOCONC | | | ISOPENTANE | 0.000 | 1.218 |
| 111 | LOMWLOCONC | | | N-PENTANE | 0.000 | 1.372 |
| 111 | LOMWLOCONC | | | N-OCTANE | 0.000 | 6.859 |
| 111 | LOMWLOCONC | | | 2-METHYL-1,3-BUTADIENE | 0.000 | 2.586 |
| 112 | NEWAIRCO84 | | | ETHYLENE | 4.800 | 3.730 |
| 112 | NEWAIRCO84 | | | PROPYLENE | 9.150 | 8.480 |
| 112 | NEWAIRCO84 | | | PROPANE | 8.610 | 7.610 |
| 112 | NEWAIRCO84 | | | TRANS-2-BUTENE | 6.920 | 7.030 |
| 112 | NEWAIRCO84 | | | ISOPENTANE | 9.850 | 9.180 |
| 112 | NEWAIRCO84 | | | TOLUENE | 9.940 | 10.920 |
| 112 | NEWAIRCO84 | | | PROPYLENE/PROPANE | 17.760 | 16.090 |
| 113 | PROPYL741 | | N415664 | PROPYLENE | 7.410 | 7.410 |
| 114 | TOLUENE211 | | | TOLUENE | 14.770 | 14.770 |
| 115 | HCHOINJ | 31-Jul-1984 | NA | FORMALDEHYDE | 1.000 | 0.946 |
| 116 | TOLUENEINJ | 28-Jun-1984 | NA | TOLUENE | 6.000 | 5.977 |
| 117 | MXYLENEINJ | 28-Jun-1984 | NA | M-XYLENE | 3.000 | 3.009 |
| 118 | AROMINJ | 16-Jul-1984 | NA | BENZENE | 2.000 | 2.000 |
| 118 | AROMINJ | 16-Jul-1984 | NA | TOLUENE | 2.000 | 2.000 |
| 118 | AROMINJ | 16-Jul-1984 | NA | P-XYLENE | 2.000 | 2.000 |
| 118 | AROMINJ | 16-Jul-1984 | NA | M-XYLENE | 2.000 | 2.000 |
| 118 | AROMINJ | 16-Jul-1984 | NA | O-XYLENE | 2.000 | 2.000 |
| 118 | AROMINJ | 16-Jul-1984 | NA | STYRENE | 2.000 | 2.000 |
| 119 | TMPENTINJ | 27-Jul-1985 | NA | 2,2,4-TRIMETHYLPENTANE | 1.000 | 1.000 |
| 120 | BENZENEINJ | 27-Jul-1984 | NA | BENZENE | 1.000 | 1.000 |
| 121 | RTIETHYL | | | ETHYLENE | 19.000 | 19.430 |
| 122 | RTIPROPYL | | | PROPYLENE | 14.400 | 14.650 |
| 123 | HIMWLIQINJ | 14-Aug-1984 | DFB | N-PENTANE | 3.000 | 2.988 |
| 123 | HIMWLIQINJ | 14-Aug-1984 | DFB | 2-METHYLPENTANE | 3.000 | 3.161 |
| 123 | HIMWLIQINJ | 14-Aug-1984 | DFB | 2,3-DIMETHYLPENTANE | 3.000 | 2.990 |
| 123 | HIMWLIQINJ | 14-Aug-1984 | DFB | TOLUENE | 3.000 | 2.988 |
| 123 | HIMWLIQINJ | 14-Aug-1984 | DFB | M-XYLENE | 3.000 | 2.973 |
| 123 | HIMWLIQINJ | 14-Aug-1984 | DFB | O-XYLENE | 2.600 | 2.663 |
| 123 | HIMWLIQINJ | 14-Aug-1984 | DFB | 2,2,4-TRIMETHYLPENTANE | 3.000 | 2.992 |
| 124 | M-XYLENE | 27-Jun-1984 | LMQ | M-XYLENE | 2.000 | 1.978 |
| 125 | HCHOINJ | 13-Jul-1984 | LMQ | FORMALDEHYDE | 1.000 | 1.038 |
| 126 | HCHOINJ | 13-Jul-1984 | LMQ | FORMALDEHYDE | 1.000 | 1.038 |
| 127 | MEOHINJ | 24-Jul-1984 | JBS | METHANOL | 0.900 | 0.891 |
| 128 | MEOHINJ | 3-Aug-1984 | DFB | METHANOL | 0.900 | 0.897 |
| 129 | MEOHINJ | 4-Aug-1984 | JRA | METHANOL | 0.300 | 0.321 |
| 130 | MEOHINJ | 7-Aug-1984 | DFB | METHANOL | 0.300 | 0.300 |
| 131 | MEOHINJ | 8-Aug-1984 | JRA | METHANOL | 0.790 | 0.787 |
| 132 | MEOHINJ | 9-Aug-1984 | LMQ | METHANOL | 0.263 | 0.263 |
| 133 | HCHOINJ | 7-Oct-1984 | NA | FORMALDEHYDE | 1.000 | 0.918 |
| 134 | HCHOINJ | 7-Oct-1984 | NA | FORMALDEHYDE | 0.500 | 0.464 |
| 135 | HCHOINJ | 9-Oct-1984 | NA | FORMALDEHYDE | 1.000 | 0.920 |
| 136 | HCHOINJ | 9-Oct-1984 | NA | FORMALDEHYDE | 1.000 | 0.920 |
| 137 | HCHOINJ | 16-Oct-1984 | NA | FORMALDEHYDE | 0.250 | 0.232 |
| 138 | HCHOINJ | 16-Oct-1984 | NA | FORMALDEHYDE | 0.500 | 0.465 |
| 139 | 85COCH4CAL | 3-Apr-1985 | AAL-15140 | METHANE | 1.907 | 1.907 |

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                    OFFICIAL CALIBRATION SOURCES               25-Sep-1985
                                                               Page 3

ID                                   SER
NUM     DESC        SDATE            NUM                                  STATED   ACTUAL
                                                                           CONC     CONC

139  85COCH4CAL    3-Apr-1985   AAL-15140    CO                           3.950    3.950
140  MEOHINJ      25-Aug-1984                METHANOL                     0.300    0.292
141  ACETALDINJ   27-Aug-1984                ACETALDEHYDE                 1.000    1.000
142  ACETALDINJ   27-Aug-1984                ACETALDEHYDE                 1.000    1.000
143  MEOHINJ       1-Sep-1984   JRA          METHANOL                     1.000    0.970
144  MEOHINJ       3-Sep-1984   KGS          METHANOL                     0.266    0.264
145  ACETALDINJ   16-Sep-1984   KGS          ACETALDEHYDE                 1.000    1.000
146  ACETALDINJ   16-Sep-1984   KGS          ACETALDEHYDE                 1.000    1.000
147  MEOHINJ      17-Sep-1984   LMQ          METHANOL                     0.600    0.572
148  HCHOINJ      25-Sep-1984   DFB          FORMALDEHYDE                 1.000    0.932
149  NO2ASPAN     20-Aug-1984   NA           PAN                          0.160    0.160
150  NO2ASPAN     20-Aug-1984   NA           PAN                          0.153    0.153
151  NO2ASPAN     18-Sep-1984   NA           PAN                          0.191    0.191
152  NO2ASPAN     18-Sep-1984   NA           PAN                          0.131    0.131
153  NO2ASPAN      3-Oct-1984   NA           PAN                          0.166    0.166
154  NO2ASPAN      3-Oct-1984   NA           PAN                          0.165    0.165
155  NO2ASPAN      4-Oct-1984   NA           PAN                          0.164    0.164
156  NO2ASPAN     11-Oct-1984   NA           PAN                          0.166    0.166
157  NO2ASPAN     30-Aug-1984   NA           PAN                          0.169    0.169
158  NO2ASPAN      6-Jul-1984   NA           PAN                          0.207    0.207
159  HCHOINJ       5-Sep-1985   NA           FORMALDEHYDE                 1.000    0.961
160  ACETINJ      15-Oct-1984   NA           ACETALDEHYDE                 1.000    1.000
161  ACETINJ      15-Oct-1984   NA           ACETALDEHYDE                 1.000    1.000
162  AROMINJ      14-May-1985   NA           BENZENE                      0.500    0.450
162  AROMINJ      14-May-1985   NA           TOLUENE                      1.000    1.005
162  AROMINJ      14-May-1985   NA           M-XYLENE                     2.000    1.999
162  AROMINJ      14-May-1985   NA           2,2,4-TRIMETHYLPENTA         2.000    1.02[illegible]
                                             NE
163  AROMINJ      17-May-1985   NA           BENZENE                      0.500    0.545
163  AROMINJ      17-May-1985   NA           TOLUENE                      1.000    1.064
163  AROMINJ      17-May-1985   NA           M-XYLENE                     2.000    2.105
163  AROMINJ      17-May-1985   NA           2,2,4-TRIMETHYLPENTA         3.000    2.349
                                             NE
164  HCHOINJ      20-May-1985   NA           FORMALDEHYDE                 1.000    1.046
165  AROMINJ      22-May-1985   NA           BENZENE                      1.500    1.659
165  AROMINJ      22-May-1985   NA           TOLUENE                      2.000    2.161
165  AROMINJ      22-May-1985   NA           M-XYLENE                     4.000    4.274
165  AROMINJ      22-May-1985   NA           O-XYLENE                     5.000    5.543
165  AROMINJ      22-May-1985   NA           1,2,4-TRIMETHYLBENZE         5.000    5.379
                                             NE
165  AORMINJ      22-May-1985   NA           2,2,4-TRIMETHYLPENTA         1.000    0.795
                                             NE
166
                                                                          0.000    0.000
166  AROMINJ      24-May-1985   NA           BENZENE                      1.500    1.613
166  AROMINJ      24-May-1985   NA           TOLUENE                      2.000    2.101
166  AROMINJ      24-May-1985   NA           M-XYLENE                     4.000    4.155
166  AROMINJ      24-May-1985   NA           O-XYLENE                     5.000    5.389
166  AROMINJ      24-May-1985   NA           2,2,4-TRIMETHYLPENTA         1.000    0.773
                                             NE
167  RTIPROPYLE    3-Jun-1985   NA           PROPYLENE                   14.400   14.645
168  RTIETHYLEN    3-Jun-1985   NA           ETHYLENE                    19.000   19.480
169  AIRCONO                    1122590      NO                          52.400   52.458
170  SCOTTNO                    BAL177       NO                          52.600   52.600
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                        OFFICIAL CALIBRATION SOURCES              25-Sep-1985
                                                                  Page 9

ID                                 SER                            STATED  ACTUAL
NUM    DESC          SDATE         NUM                            CONC    CONC

171  LOWNOAUTO                              NO                    0.000   0.283
172  LOWNOAUTO2                             NO                    0.693   0.663
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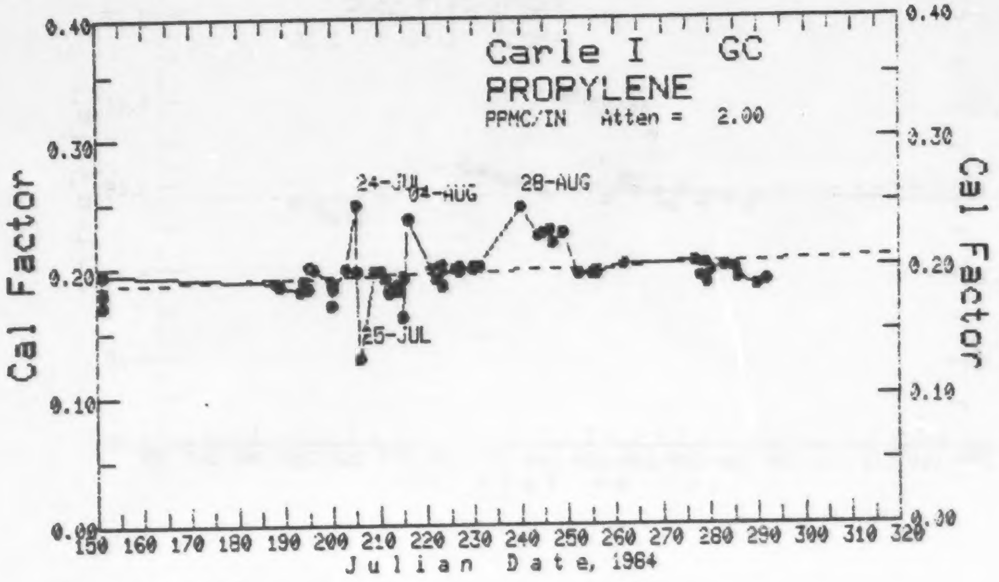
# D

# CALANA Plots and Reports



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For the species PROPYLENE and the instrument Carle I   GC:

Beginning Caldate:            30-MAY-84
                        Day:  150
Ending    Caldate:            16-NOV-84
                        Day:  320
Upper CalFactor Limit            0.40000
Lower CalFactor Limit            0.00000

The number of data points        62
The number included  was         62
The slope of this fit  is 1.3522654E-004
      with a std dev of 6.6911662E-005   rel. dev = 49.5 %
The intercept is          1.6694184E-001
      with a std dev of 1.5341250E-002   rel. dev = 9.2 %
The std dev of the fit is 1.8079919E-002   PE =  0.01205
The correlation coeff is   0.25246

The min, mean, max are        0.13040,     0.19760,     0.25009
The standard deviation is  0.01853   rel. dev = 9.4 %

Cal =  0.00014 X (Julian Date - 150) +  0.18723

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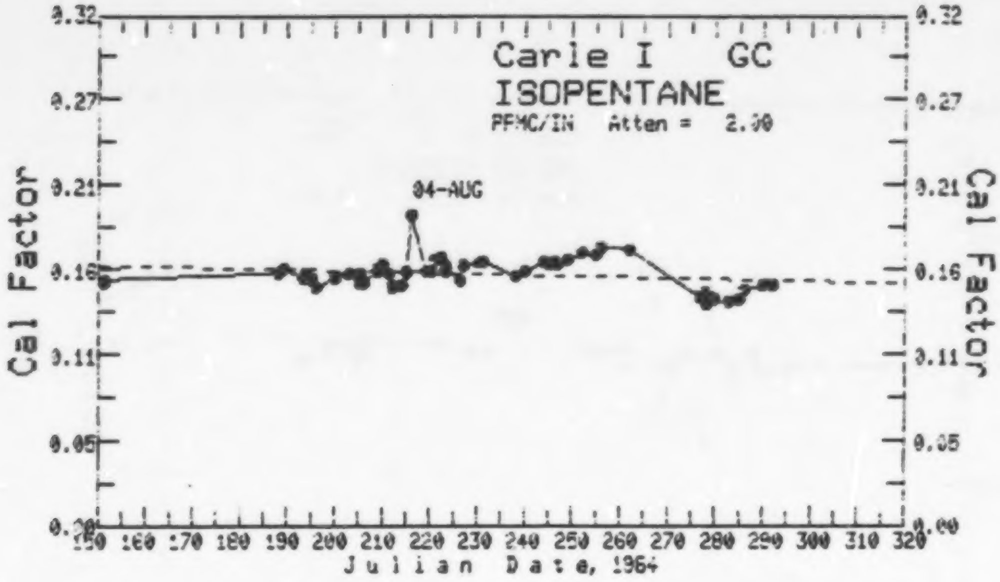

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For the species ISOPENTANE and the instrument Carle I   GC:

Beginning Caldate:          30-MAY-84
                      Day:  150
Ending    Caldate:          16-NOV-84
                      Day:  320
Upper CalFactor Limit          0.32000
Lower CalFactor Limit          0.00000

The number of data points      61
The number included  was       61
The slope of this fit  is -6.274875E-005
       with a std dev of  3.6480040E-005    rel. dev = -58.1 %
The intercept is          1.7246965E-001
       with a std dev of  8.4102093E-003    rel. dev = 4.9 %
The std dev of the fit is 9.7288922E-003    PE =  0.00649
The correlation coeff is  -0.21852

The min, mean, max are         0.13965,     0.15816,     0.19620
The standard deviation is  0.00989   rel. dev = 6.3 %

Cal = -0.00006 X (Julian Date - 150) +  0.16306
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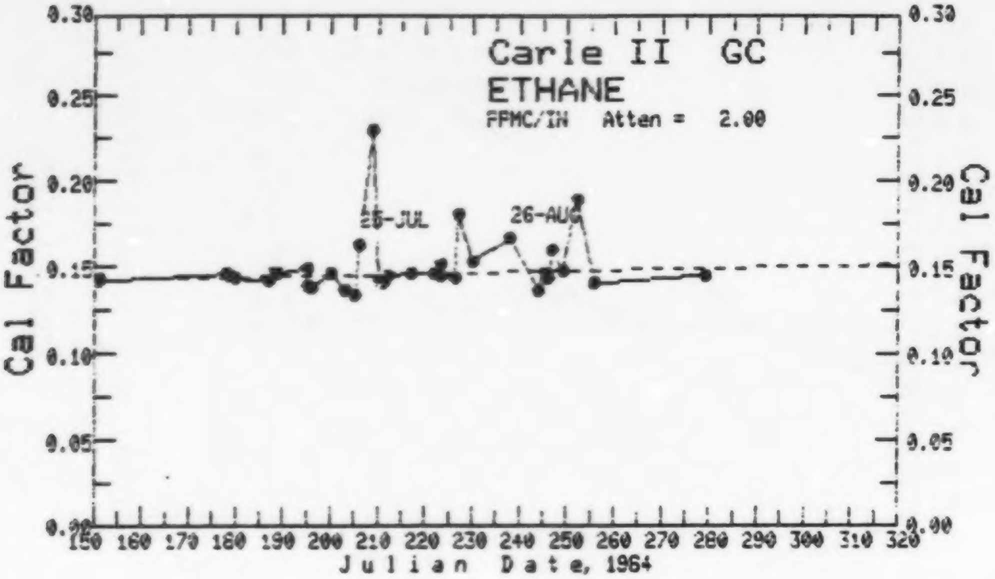

```
For the species ETHANE and the instrument Carle II  GC:

Beginning Caldate:          30-MAY-84
                      Day:  150
Ending     Caldate:         16-NOV-84
                      Day:  320
Upper CalFactor Limit          0.18000
Lower CalFactor Limit          0.00000

The number of data points      35
The number included  was       32
The slope of this fit  is 5.6237375E-005
       with a std dev of 4.3453789E-005    rel. dev = 77.3 %
The intercept is          1.3469188E-001
       with a std dev of 9.2956360E-003    rel. dev = 6.9 %
The std dev of the fit is 7.1982245E-003   PE =  0.00480
The correlation coeff is   0.22995

The min, mean, max are        0.13445,    0.14661,    0.23050
The standard deviation is  0.00728   rel. dev = 5.0 %

Cal =  0.00006 X (Julian Date - 150) +  0.14313
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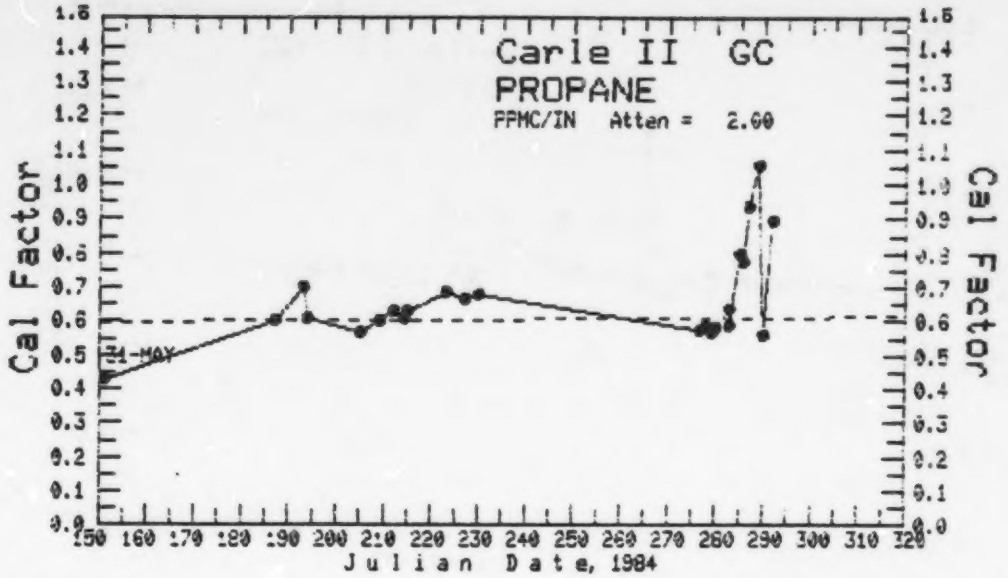

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For the species PROPANE and the instrument Carle II  GC:

Beginning Caldate:          30-MAY-84
                      Day:  150
Ending    Caldate:          16-NOV-84
                      Day:  320
Upper CalFactor Limit          0.70000
Lower CalFactor Limit          0.00000

The number of data points      24
The number included  was       19
The slope of this fit  is 9.3254754E-005
        with a std dev of 3.4843816E-004   rel. dev = 373.6 %
The intercept is          5.8478932E-001
        with a std dev of 8.2456137E-002   rel. dev = 14.1 %
The std dev of the fit is 6.1473938E-002   PE =  0.04098
The correlation coeff is   0.06478

The min, mean, max are       0.42750,    0.60653,    1.05930
The standard deviation is  0.05987   rel. dev = 9.9 %

Cal =  0.00009 X (Julian Date - 150) +  0.59878
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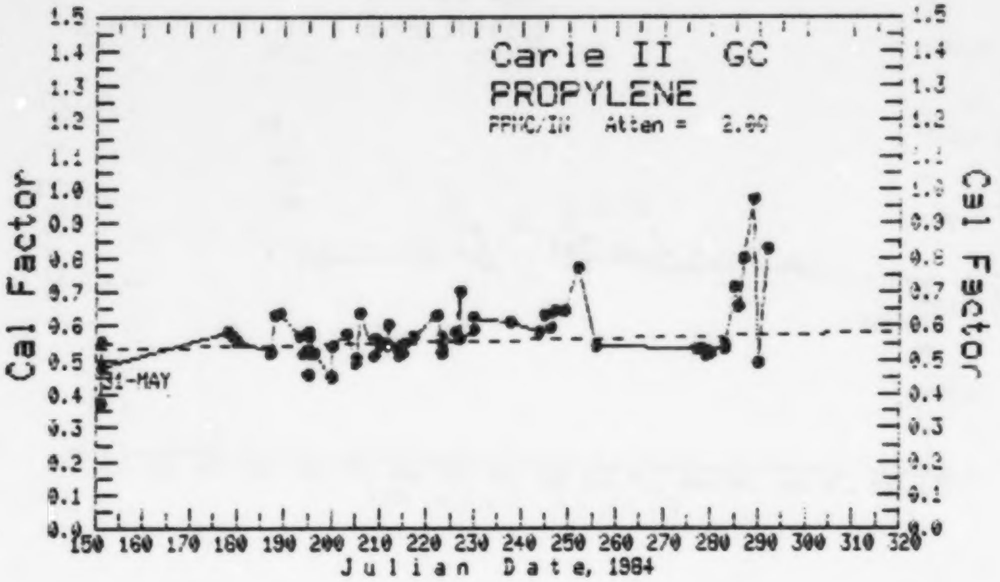

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For the species PROPYLENE and the instrument Carle II  GC:

Beginning Caldate:          30-MAY-84
                      Day:  150
Ending    Caldate:          16-NOV-84
                      Day:  320
Upper CalFactor Limit          0.70000
Lower CalFactor Limit          0.00000

The number of data points      63
The number included  was       57
The slope of this fit  is 3.2677424E-004
        with a std dev of 2.0339685E-004   rel. dev = 62.2 %
The intercept is          4.8080472E-001
        with a std dev of 4.5272312E-002   rel. dev = 9.4 %
The std dev of the fit is 5.3626706E-002   PE =  0.03575
The correlation coeff is   0.21172

The min, mean, max are        0.36888,    0.55264,    0.97565
The standard deviation is  0.05438   rel. dev = 9.8 %

Cal =  0.00033 X (Julian Date - 150) +  0.52982

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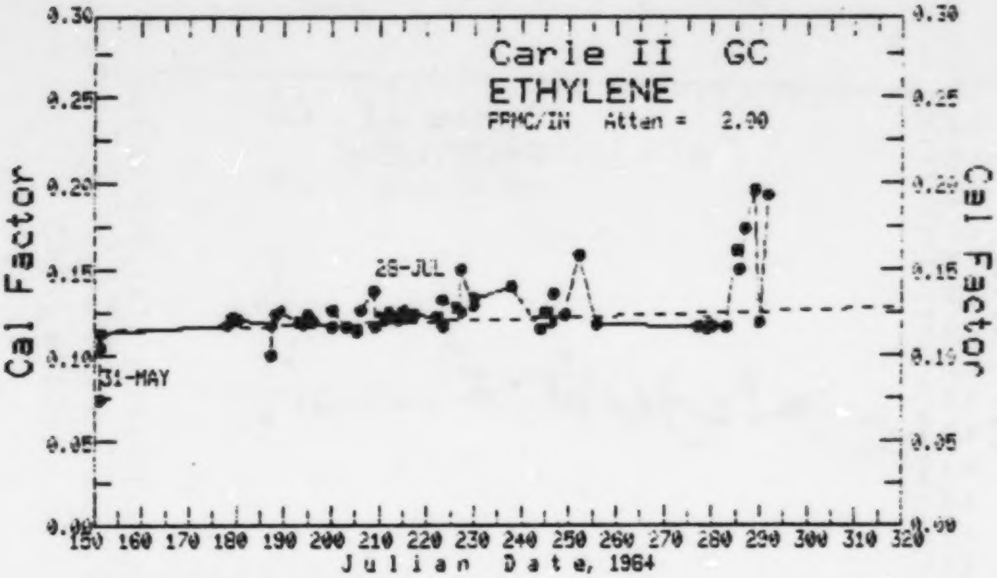

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For the species ETHYLENE and the instrument Carle II  GC:

Beginning Caldate:          30-MAY-84
                   Day:     150
Ending    Caldate:          16-NOV-84
                   Day:     320
Upper CalFactor Limit          0.14000
Lower CalFactor Limit          0.00000

The number of data points     61
The number included  was       53
The slope of this fit  is 7.7424523E-005
       with a std dev of 3.6302085E-005   rel. dev = 46.9 %
The intercept is          1.0432247E-001
       with a std dev of 7.9898236E-003   rel. dev = 7.7 %
The std dev of the fit is 8.8857276E-003   PE =  0.00592
The correlation coeff is   0.28616

The min, mean, max are        0.07444,    0.12116,    0.19795
The standard deviation is  0.00918   rel. dev = 7.6 %

Cal =  0.00008 X (Julian Date - 150) +  0.11594

                      ...press RETURN-key when ready...
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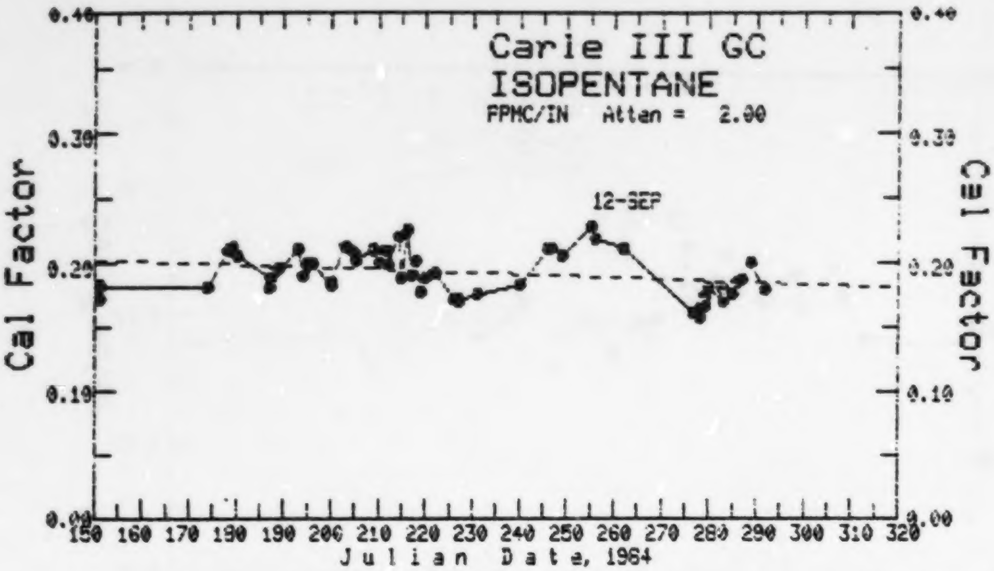

```
For the species ISOPENTANE and the instrument Carle III GC:

Beginning Caldate:            30-MAY-84
                     Day:     150
Ending    Caldate:            16-NOV-84
                     Day:     320
Upper CalFactor Limit             0.40000
Lower CalFactor Limit             0.00000

The number of data points     60
The number included  was      60
The slope of this fit  is -1.222656E-004
       with a std dev of 5.6003271E-005   rel. dev = -45.8 %
The intercept is          2.2209272E-001
       with a std dev of 1.2738738E-002   rel. dev = 5.7 %
The std dev of the fit is 1.6698649E-002   PE =  0.01113
The correlation coeff is  -0.27557

The min, mean, max are       0.15986,    0.19468,    0.23074
The standard deviation is  0.01722   rel. dev = 8.8 %

Cal = -0.00012 X (Julian Date - 150) +  0.20375

                     ...press RETURN-key when ready...
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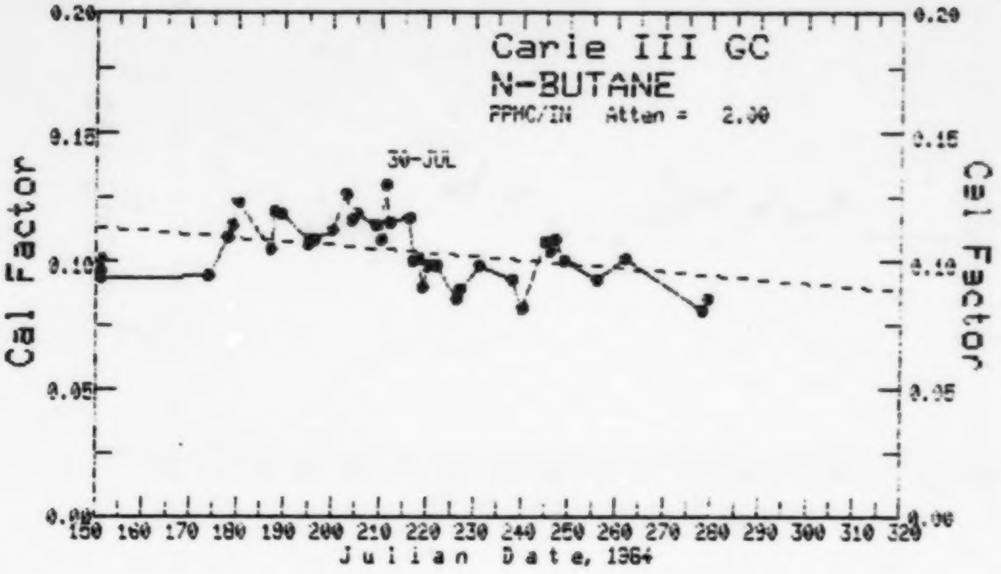


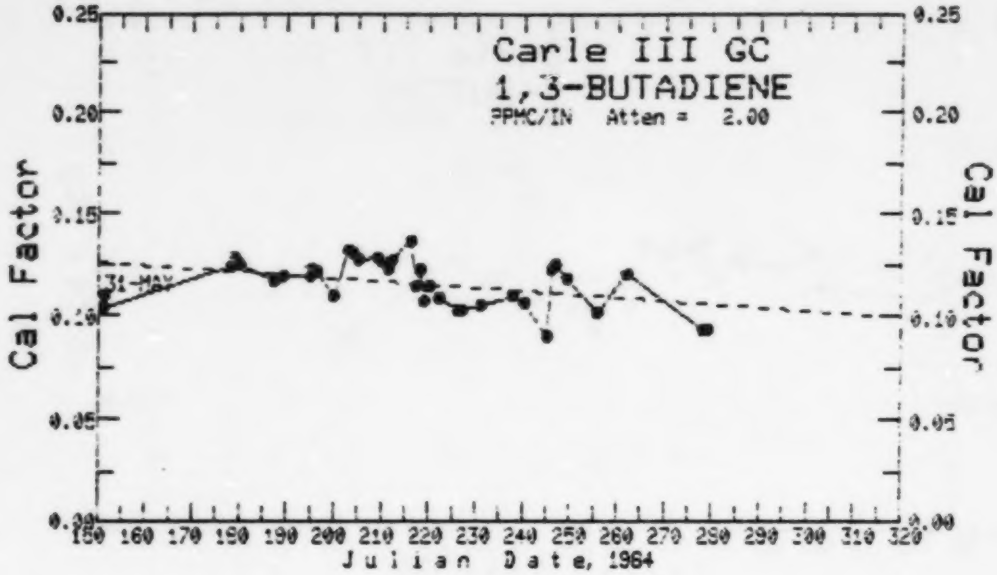
```
For the species N-BUTANE and the instrument Carle III GC:

Beginning Caldate:          30-MAY-84
                  Day:      150
Ending     Caldate:         16-NOV-84
                  Day:      320
Upper CalFactor Limit          0.20000
Lower CalFactor Limit          0.00000

The number of data points      40
The number included  was       40
The slope of this fit  is  -1.501925E-004
       with a std dev of  5.7705246E-005    rel. dev = -38.4 %
The intercept is           1.3697557E-001
       with a std dev of  1.2401192E-002    rel. dev = 9.1 %
The std dev of the fit is  1.1458466E-002   PE =  0.00764
The correlation coeff is  -0.38897

The min, mean, max are         0.08147,    0.10504,    0.13079
The standard deviation is  0.01228    rel. dev = 11.7 %

Cal = -0.00015 X (Julian Date - 150) +  0.11445
```



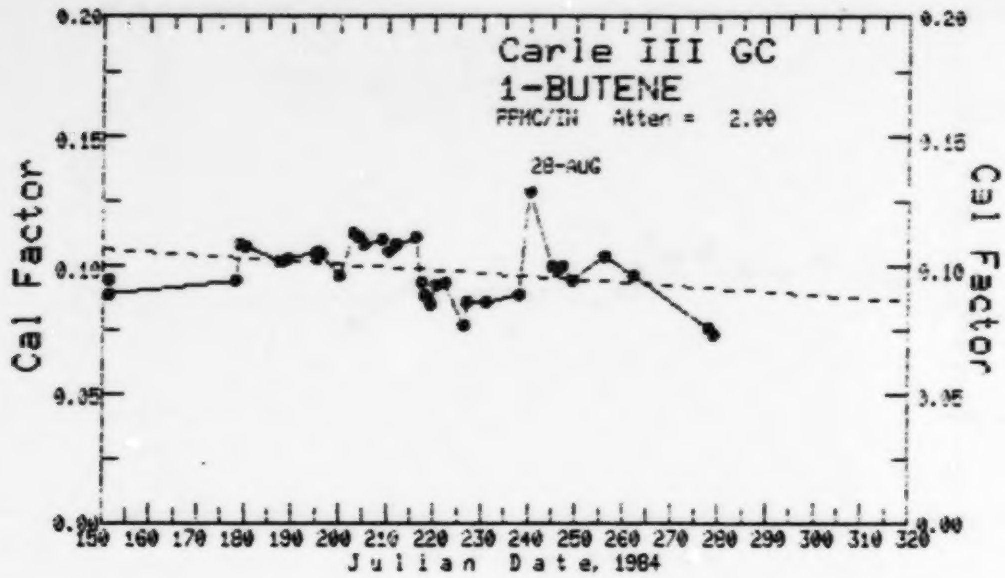
```
For the species 1,3-BUTADIENE and the instrument Carle III GC:

Beginning Caldate:           30-MAY-84
                   Day:      150
Ending    Caldate:           16-NOV-84
                   Day:      320
Upper CalFactor Limit            0.25000
Lower CalFactor Limit            0.00000

The number of data points        38
The number included  was         38
The slope of this fit  is -1.547570E-004
         with a std dev of 5.7985070E-005    rel. dev = -37.5 %
The intercept is           1.4937310E-001
         with a std dev of 1.2600050E-002    rel. dev = 8.4 %
The std dev of the fit is 1.0673171E-002    PE =  0.00712
The correlation coeff is  -0.40642

The min, mean, max are        0.09043,     0.11606,     0.13717
The standard deviation is  0.01152   rel. dev = 9.9 %

Cal = -0.00015 X (Julian Date - 150) +  0.12616
```



```
For the species 1-BUTENE and the instrument Carle III GC:

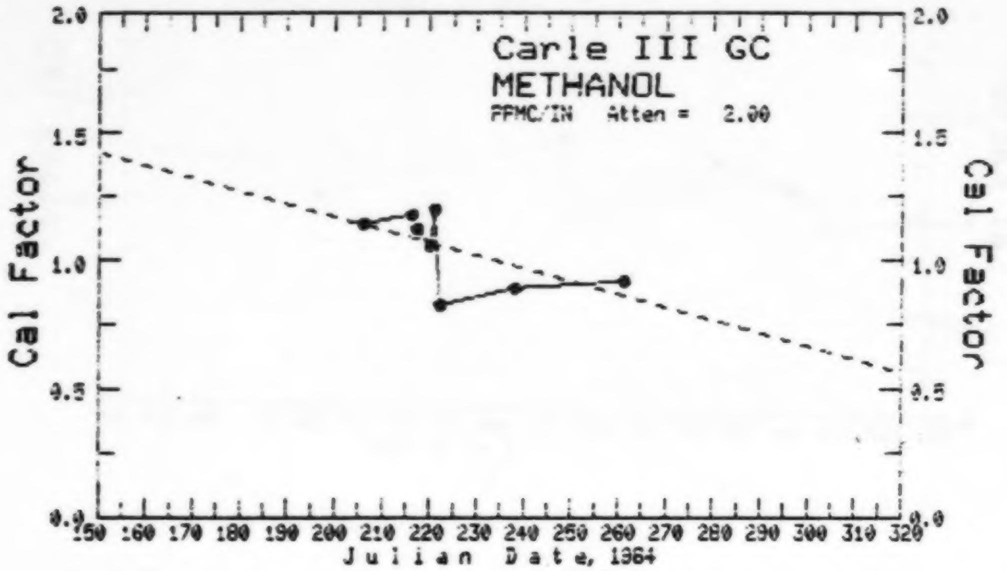
Beginning Caldate:          30-MAY-84
                       Day:  150
Ending     Caldate:          16-NOV-84
                       Day:  320
Upper CalFactor Limit          0.20000
Lower CalFactor Limit          0.00000

The number of data points      38
The number included  was       38
The slope of this fit  is -1.182031E-004
       with a std dev of 5.9781057E-005   rel. dev = -50.6 %
The intercept is          1.2497382E-001
       with a std dev of 1.2990315E-002   rel. dev = 10.4 %
The std dev of the fit is 1.1003754E-002   PE =  0.00734
The correlation coeff is   -0.31299

The min, mean, max are        0.07366,     0.09953,     0.12998
The standard deviation is  0.01143   rel. dev = 11.5 %

Cal = -0.00012 X (Julian Date - 150) +  0.10724

                     ...press RETURN-key when ready...
```



```
For the species METHANOL and the instrument Carle III GC:

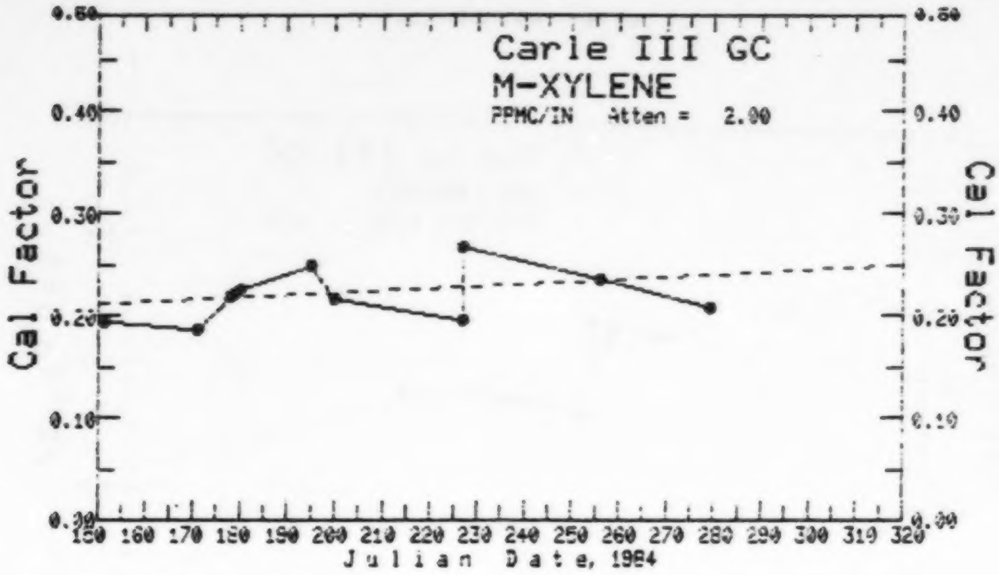
Beginning Caldate:          30-MAY-84
                  Day:      150
Ending    Caldate:          16-NOV-84
                  Day:      320
Upper CalFactor Limit          2.00000
Lower CalFactor Limit          0.00000

The number of data points      8
The number included  was       8
The slope of this fit  is -5.071507E-003
       with a std dev of 2.7547702E-003    rel. dev = -54.3 %
The intercept is          2.1918042E+000
       with a std dev of 6.2171127E-001    rel. dev = 28.4 %
The std dev of the fit is 1.2383833E-001    PE =  0.08256
The correlation coeff is  -0.60081

The min, mean, max are       0.83510,     1.05008,     1.20625
The standard deviation is  0.14342   rel. dev = 13.7 %

Cal = -0.00507 X (Julian Date - 150) +  1.43108

                    ...press RETURN-key when ready...
```



```
For the species M-XYLENE and the instrument Carle III GC:

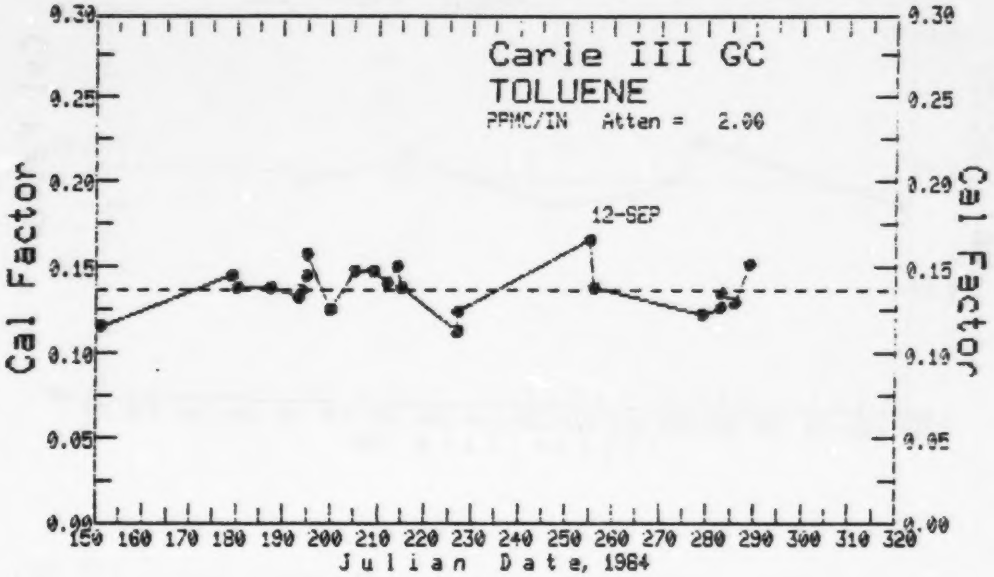
Beginning Caldate:          30-MAY-84
                    Day:    150
Ending     Caldate:         16-NOV-84
                    Day:    320
Upper CalFactor Limit          0.50000
Lower CalFactor Limit          0.00000

The number of data points      12
The number included  was       12
The slope of this fit  is 2.2924388E-004
       with a std dev of 2.1399147E-004   rel. dev = 93.3 %
The intercept is          1.7734365E-001
       with a std dev of 4.4723535E-002   rel. dev = 25.2 %
The std dev of the fit is 2.6853727E-002   PE =  0.01790
The correlation coeff is   0.32086

The min, mean, max are       0.18690,     0.22453,     0.26853
The standard deviation is  0.02703   rel. dev = 12.0 %

Cal =  0.00023 X (Julian Date - 150) +  0.21173

                      ...press RETURN-key when ready...
```



```
For the species TOLUENE and the instrument Carle III GC:

Beginning Caldate:          30-MAY-84
                      Day:  150
Ending    Caldate:          16-NOV-84
                      Day:  320
Upper CalFactor Limit          0.30000
Lower CalFactor Limit          0.00000

The number of data points      25
The number included  was       25
The slope of this fit  is 9.4526308E-007
       with a std dev of 7.3484704E-005   rel. dev = 7774.0 %
The intercept is          1.3672349E-001
       with a std dev of 1.6525408E-002   rel. dev = 12.1 %
The std dev of the fit is 1.3980213E-002   PE =  0.00932
The correlation coeff is    0.00268

The min, mean, max are       0.11350,    0.13693,    0.16721
The standard deviation is  0.01369   rel. dev = 10.0 %

Cal =  0.00000 X (Julian Date - 150) +  0.13687

                      ...press RETURN-key when ready...
```

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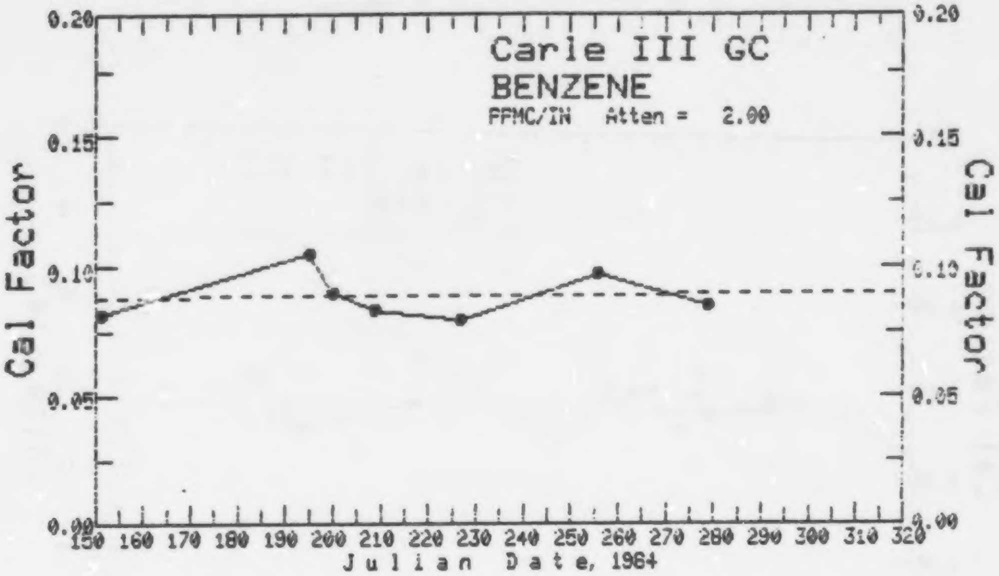


```
For the species BENZENE and the instrument Carle III GC:

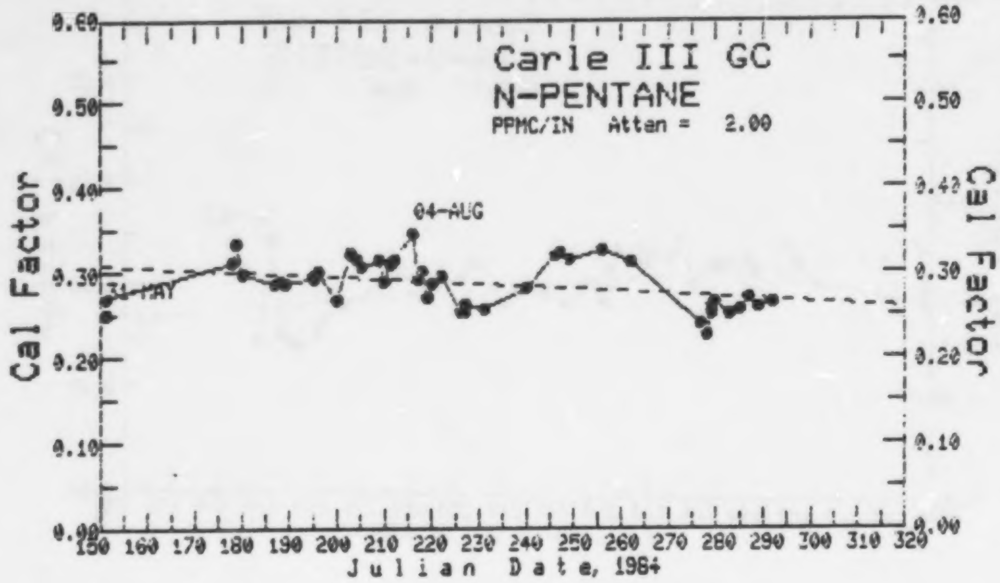
Beginning Caldate:          30-MAY-84
                  Day:      150
Ending    Caldate:          16-NOV-84
                  Day:      320
Upper CalFactor Limit          0.20000
Lower CalFactor Limit          0.00000

The number of data points      7
The number included  was       7
The slope of this fit  is 1.0564688E-005
        with a std dev of 9.7659602E-005   rel. dev = 924.4 %
The intercept is          8.7323874E-002
        with a std dev of 2.1504541E-002   rel. dev = 24.6 %
The std dev of the fit is 1.0081872E-002   PE =  0.00672
The correlation coeff is   0.04832

The min, mean, max are        0.08022,    0.08961,    0.10564
The standard deviation is  0.00921   rel. dev = 10.3 %

Cal =  0.00001 X (Julian Date - 150) +  0.08891

                    ...press RETURN-key when ready...
```



```
For the species N-PENTANE and the instrument Carle III GC:

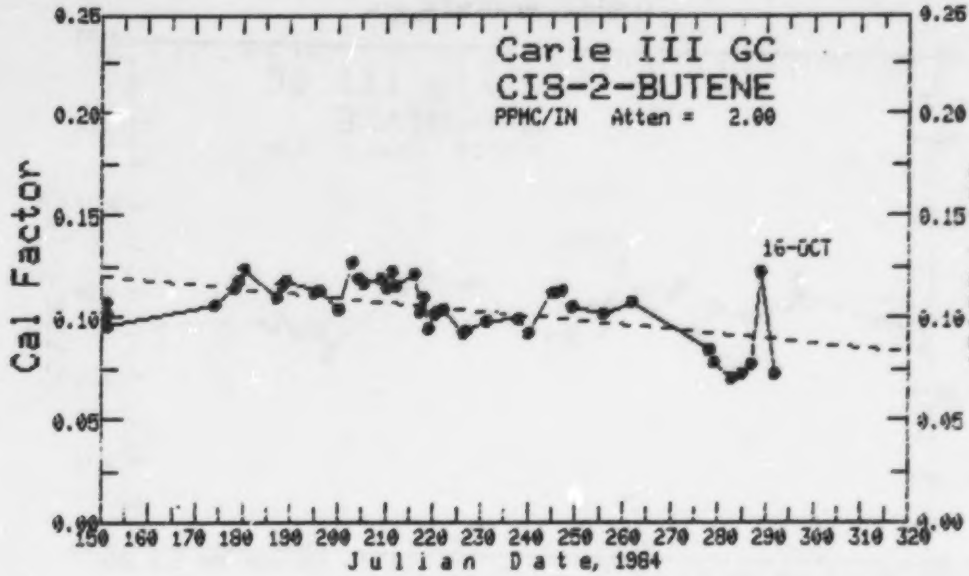
Beginning Caldate:         30-MAY-84
                     Day:  150
Ending    Caldate:         16-NOV-84
                     Day:  320
Upper CalFactor Limit        0.60000
Lower CalFactor Limit        0.00000

The number of data points    45
The number included  was     45
The slope of this fit  is -2.873216E-004
      with a std dev of 1.0329445E-004   rel. dev = -36.0 %
The intercept is          3.5367520E-001
      with a std dev of 2.3728269E-002   rel. dev = 6.7 %
The std dev of the fit is 2.6308086E-002   PE =  0.01754
The correlation coeff is  -0.39051

The min, mean, max are       0.22760,    0.28858,    0.34680
The standard deviation is  0.02825   rel. dev = 9.8 %

Cal = -0.00029 X (Julian Date - 150) +  0.31058

                   ...press RETURN-key when ready...
```



```
For the species CIS-2-BUTENE and the instrument Carle III GC:

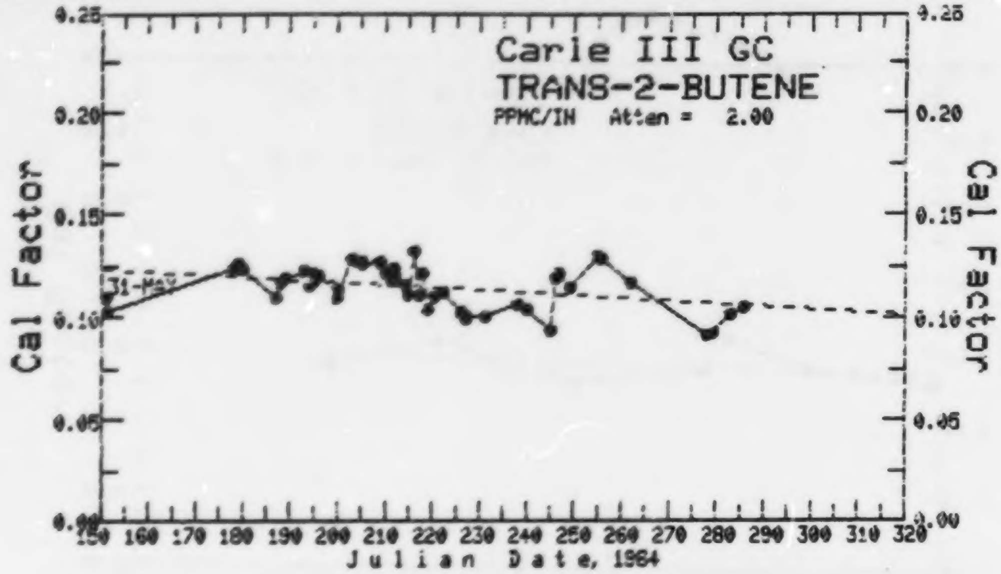
Beginning Caldate:          30-MAY-84
                      Day:  150
Ending    Caldate:          16-NOV-84
                      Day:  320
Upper CalFactor Limit          0.35000
Lower CalFactor Limit          0.00000

The number of data points      45
The number included  was       45
The slope of this fit  is -2.188447E-004
      with a std dev of 4.8220399E-005   rel. dev = -22.0 %
The intercept is           1.5340966E-001
      with a std dev of 1.0805980E-002   rel. dev = 7.0 %
The std dev of the fit is 1.2219133E-002   PE =  0.00815
The correlation coeff is  -0.56910

The min, mean, max are        0.07010,    0.10507,    0.12707
The standard deviation is  0.01469   rel. dev = 14.0 %

Cal = -0.00022 X (Julian Date - 150) +  0.12058

                      ...press RETURN-key when ready...
```



```
For the species TRANS-2-BUTENE and the instrument Carle III GC:

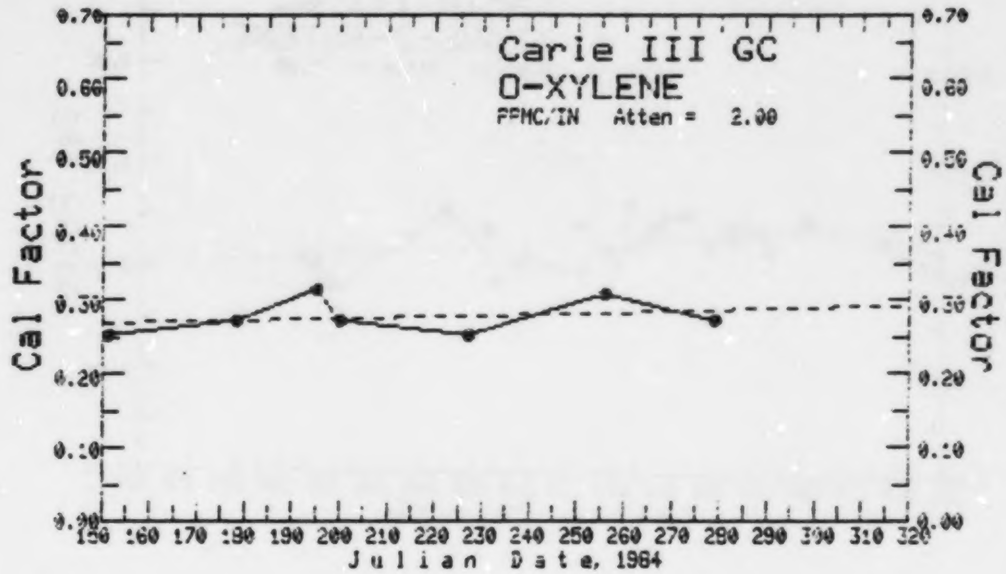
Beginning Caldate:             30-MAY-84
                         Day:  150
Ending     Caldate:            16-NOV-84
                         Day:  320
Upper CalFactor Limit             0.30000
Lower CalFactor Limit             0.00000

The number of data points         50
The number included  was          50
The slope of this fit  is -1.273805E-004
        with a std dev of 4.6032130E-005   rel. dev = -36.1 %
The intercept is          1.4263830E-001
        with a std dev of 1.0106748E-002   rel. dev = 7.1 %
The std dev of the fit is 9.9038982E-003   PE =  0.00660
The correlation coeff is  -0.37092

The min, mean, max are        0.09145,    0.11494,    0.13217
The standard deviation is  0.01056   rel. dev = 9.2 %

Cal = -0.00013 X (Julian Date - 150) +  0.12353

                    ...press RETURN-key when ready...
```



```
For the species O-XYLENE and the instrument Carle III GC:

Beginning Caldate:          30-MAY-84
                      Day:  150
Ending    Caldate:          16-NOV-84
                      Day:  320
Upper CalFactor Limit          0.70000
Lower CalFactor Limit          0.00000

The number of data points       7
The number included  was        7
The slope of this fit  is 1.3699588E-004
      with a std dev of 2.3682240E-004   rel. dev = 172.9 %
The intercept is          2.5194653E-001
      with a std dev of 5.1218128E-002   rel. dev = 20.3 %
The std dev of the fit is 2.5898701E-002   PE =  0.01727
The correlation coeff is    0.25046

The min, mean, max are       0.25603,     0.28103,     0.31762
The standard deviation is  0.02442   rel. dev = 8.7 %

Cal =  0.00014 X (Julian Date - 150) +  0.27250
```

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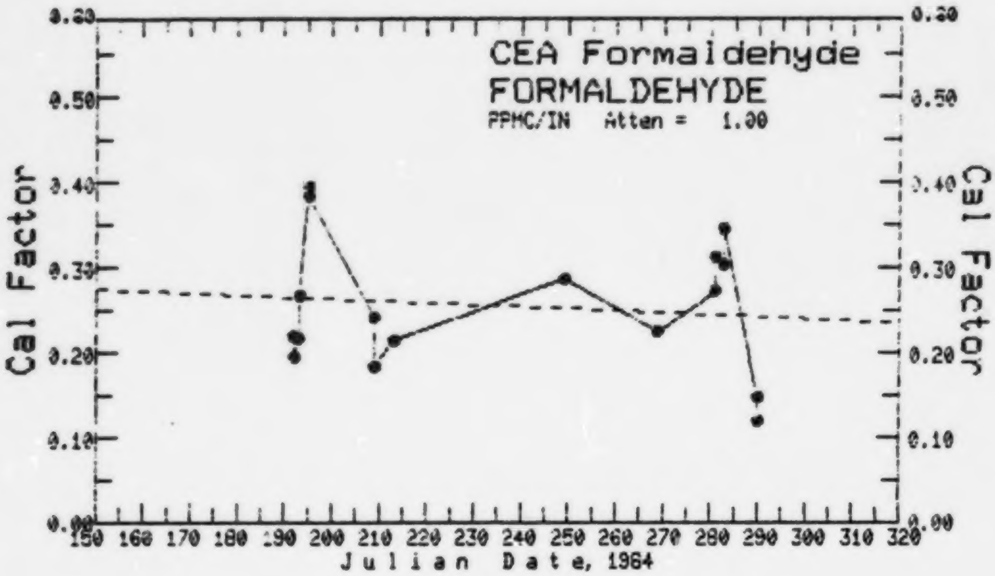

```
For the species FORMALDEHYDE and the instrument CEA Formaldehyde:

Beginning Caldate:          30-MAY-84
                     Day:   150
Ending    Caldate:          16-NOV-84
                     Day:   320
Upper CalFactor Limit          0.60000
Lower CalFactor Limit          0.00000

The number of data points      17
The number included  was       17
The slope of this fit  is -2.282711E-004
      with a std dev of 4.7236958E-004    rel. dev = -206.9 %
The intercept is          3.1092736E-001
      with a std dev of 1.1328004E-001    rel. dev = 36.4 %
The std dev of the fit is 7.9710921E-002  PE =  0.05314
The correlation coeff is  -0.12381

The min, mean, max are         0.12160,    0.25699,    0.39930
The standard deviation is  0.07778   rel. dev = 30.3 %

Cal = -0.00023 X (Julian Date - 150) +  0.27669

                     ...press RETURN-key when ready...
```